SpectraSuite
Spectrometer Operating Software

Installation and Operation Manual

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About This Manual

Document Purpose and Intended Audience

This document provides you with an installation and configuration instructions to get your system up and running. In addition, user interface for SpectraSuite is provided.

What's New in this Document

This version of the *SpectraSuite Spectrometer Operating Software Installation and Operation Manual* adds the SeaChanger module.

Document Summary

Chapter	Description
Chapter 1: *Introduction*	Provides an overview of the SpectraSuite operating software.
Chapter 2: *Installation*	Contains instructions for installing and configuring the SpectraSuite software.
Chapter 3: *Controls and Indicators*	Illustrates options for customizing your graph view. Also contains information for peak finding.
Chapter 4: *File Menu Functions*	Contains descriptions of the functions on the File menu.
Chapter 5: *View Menu Functions*	Contains a description of the functions on the View menu.
Chapter 6: *Spectrometer Menu Functions*	Contains descriptions of the functions on the Spectrometer menu.
Chapter 7: *Processing Menu Functions*	Contains descriptions of the functions on the Processing menu.
Chapter 8: *Tools Menu Functions*	Discusses the selections available in the Tools menu.
Chapter 9: *Window Menu Functions*	Contains information for the Window menu functions.
Chapter 10: *Strip Charts*	Provides instructions for using the Strip Charts feature.

Chapter	Description
Appendix A: *Experiment Tutorials*	Contains instructions for performing sample experiments using an Ocean Optics spectrometer and SpectraSuite software.
Appendix B: *Troubleshooting*	Provides a table of possible problems and suggested solutions.

Product-Related Documentation

External Triggering Options

Various USB spectrometer documents such as the *USB4000 Spectrometer Installation and Operation Manual*.

ADC1000-USB Operating Instructions

SeaChanger 4-Channel Installation and Operation Manual

SeaChanger Wash 4-Channel Color Engine Installation and Operation Manual

You can access documentation for Ocean Optics products by visiting our website at http://www.oceanoptics.com. Select *Technical → Operating Instructions*, then choose the appropriate document from the available drop-down lists. Or, use the **Search by Model Number** field at the bottom of the web page.

You can also access operating instructions for Ocean Optics products on the *Software and Technical Resources* CD included with the system.

Engineering-level documentation is located on our website at *Technical → Engineering Docs.*

Upgrades

Occasionally, you may find that you need Ocean Optics to make a change or an upgrade to your system. To facilitate these changes, you must first contact Customer Support and obtain a Return Merchandise Authorization (RMA) number. Please contact Ocean Optics for specific instructions when returning a product.

Chapter 1

Introduction

Product Overview

SpectraSuite is a completely modular, Java-based spectroscopy software platform that operates on Windows, Macintosh and Linux operating systems. The software can control any Ocean Optics USB spectrometer and device, as well as any other manufacturer's USB instrumentation using the appropriate drivers. The SpectraSuite interface looks and feels the same on all operating systems yet retains the familiar appearance of an application native to each OS. Ocean Optics is the first to offer such a flexible, feature-packed application with this level of cross-platform capability.

The SpectraSuite Java-based framework is modular and every function in it can be altered or replaced. For instance, the data acquisition functions, the scheduling functions, the data processing functions and the rendering functions are all separate modules. You can add or delete modules to create a proprietary user interface or functionality; create modules to perform calculations; automate experiment routines and more. You or an Ocean Optics application developer can easily customize SpectraSuite through Java code.

SpectraSuite is the platform for all future Ocean Optics application software development. Current software applications including OOISensors and OOILIBS will be migrated to the SpectraSuite platform in the near future.

USB Spectrometer and Device Control

SpectraSuite easily manages multiple USB spectrometers – each with different acquisition parameters – in multiple windows, and provides graphical and numeric representation of spectra from each spectrometer. Using SpectraSuite, you can combine data from multiple sources for applications that include upwelling/downwelling measurements, dual-beam referencing and process monitoring.

SpectraSuite can be used with the following Ocean Optics spectrometers when they are interfacing to a computer through their USB port:

S2000 Spectrometer (with A/D Converter)

USB650 Spectrometer

USB2000 Spectrometer

USB2000+ Spectrometer

USB2000-FLG Spectrometer

USB4000 Spectrometer

HR2000 High-resolution Spectrometer

HR2000+High-resolution Spectrometer

HR4000 High-resolution Spectrometer

QE65000 Scientific-grade Spectrometer

NIR-512 Near-IR Spectrometer

NIR256-2.1 and NIR256-2.5 Near-IR Spectrometers

MMS Raman Spectrometer

In addition, SpectraSuite also supports the following USB devices:

ADC1000-USB A/D Converter

Spectral Hyper Adapter (SHA-1)

Features

Modular Framework – The SpectraSuite framework is modular and every function in it can be altered or replaced. For instance, the data acquisition functions, the scheduling functions, the data processing functions and the rendering functions are all separate modules. You can add or delete modules to create a proprietary user interface or functionality; create modules to perform calculations; automate experiment routines, and more. You or an Ocean Optics application developer can easily customize SpectraSuite through Java code.

Platform Independent – The SpectraSuite is a platform-independent application that provides Graphical and numeric representation of spectra in one window. SpectraSuite can operate on a Windows, Linux, or Macintosh operating system.

Advanced Data Capture Control – SpectraSuite provides the user with advanced control of episodic data capture attributes. For instance, a user can acquire data for a fixed number of scans or for a specific interval. Initiation of each scan can be externally triggered or event-driven. Captured data is quickly stored into a systems memory at speeds as fast as 1 scan per msec with speeds limited by hardware performance.

Independent Control of Multiple USB Devices – Multiple USB devices can be monitored on the same graph in a single window; each of these devices can be controlled independently.

SpectraSuite in the Future

SpectraSuite is constantly evolving. With the purchase of SpectraSuite, you are entitled to one year of free, web-based, automatic upgrades (see *Getting Updates*).

Planned future enhancements include the following:

21 CFR Part 11 Compliant – SpectraSuite will be 21 CFR Part 11 compliant with an encoded binary file. This binary data format tracks the complete history of all processing steps that are performed on the data. Spectra suite stores and provides data in a variety of other formats including tab-delimited ASCII (for Excel or other analysis packages), Grams SPC, and JCAMP. Additionally, Spectra Suite offers a database module where arbitrary data can be stored in any user-selectable format. Another benefit of the software's binary data tracking function is that it offers a user "process do-overs." A user can change the values of various parameters in a process and apply those changes to data without having to recreate an entire process.

Fully Internationalized – All of the software's menus, dialog boxes, prompts, messages and files will be able to reflect a native language by simply changing a single file. Modules that support Japanese, Chinese, Korean and Spanish will be available in the near future, followed by French, German and Italian.

Spectroscopic Functions

SpectraSuite allows you to perform the three basic spectroscopic experiments – absorbance, reflectance and emission – as well as signal-processing functions such as electrical dark-signal correction, stray light correction, boxcar pixel smoothing and signal averaging. Scope mode, the spectrometer operating mode in which raw data (signal) is acquired by the detector, allows you to establish these signal-conditioning parameters. The basic concept for the software is that real-time display of data allows users to evaluate the effectiveness of their experimental setups and data processing selections, make changes to these parameters, instantly see the effects and save the data. Most spectrometer-system operating software does not allow such signal-conditioning flexibility.

With SpectraSuite, you can perform time-acquisition experiments for kinetics applications. As part of the time-acquisition function (strip charts), you can monitor and report up to 6 single wavelengths and up to 2 mathematical combinations of these wavelengths. In addition, you can perform reference monitoring in a variety of ways: single wavelength (1 or 2 channels), integrated intensity (starting and ending wavelengths for 1 or 2 channels) and wavelength-by-wavelength (2 channels).

SpectraSuite gives you complete control of setting the parameters for all system functions such as acquiring data, designing the graph display, and using spectra overlays. You can also save and then retrieve all of these system parameters for future experiments. SpectraSuite has the benefit of providing various software-controlled triggering options for external events such as laser firing or light source pulsing.

Other advanced features give you several data-collection options. You can independently store and retrieve dark, reference, sample and processed spectra. All data can be saved to disk using autoincremented filenames. You can save data as ASCII files or in the native GRAMS/32 SPC or JCAMP format. One feature prints the spectra and another copies spectral data into other software such as Excel and Word.

Getting Updates

SpectraSuite software features one year of free, web-based automatic upgrades when you buy the software. This service requires that you register the first time you connect. You can purchase renewals for half the software price per year. All customers (whether they have a free upgrade plan or not) will be able to get free bug fixes.

The update icon ( ) appears on the lower right corner of the SpectraSuite screen when updates are available for your software (see *Update Available* for more information on this icon). Click on this icon, or select **Tools | Update Center** from the SpectraSuite menu to go to the Update Center. Follow the steps in the Update Center wizard to update your SpectraSuite software.

Chapter 2

Installation

Overview

The following sections will guide you in installing SpectraSuite on a Windows, Macintosh or Linux operating system.

Note

Do NOT connect the spectrometer to the computer until you install the SpectraSuite software. Follow the instructions contained in this chapter to properly connect and configure your system.

Installing SpectraSuite

SpectraSuite can be downloaded from the Ocean Optics ftp site, or retrieved from the CD that you received with your purchase of the software.

This section contains instructions for installing SpectraSuite using both methods on each of the following operating systems:

Microsoft Windows – Windows 2000, XP

Apple Macintosh – OS X version 10.0 or later

Linux – Red Hat 9 or later, Fedora (any version), Debian 3.1 (Sarge), and SUSE (9.0 or later)

Retrieving from a CD

Your SpectraSuite software is shipped to you from Ocean Optics on a CD. The software is located either on the main **Software and Technical Resources** CD, or on a separate CD labeled **SpectraSuite Spectroscopy Platform Software**. You will need the password located on the jacket of the CD containing your SpectraSuite software to complete the installation.

► *Procedure*

1. Insert the CD that you received containing your SpectraSuite software into your computer.
2. Select the SpectraSuite software for your computer's operating platform via the CD interface. Then follow the prompts in the installation wizard.

   Or,

   Browse to the appropriate SpectraSuite set-up file for your computer and double-click it to start the software installation. Set-up files are as follows:

   - Windows: SpectraSuiteSetup_Windows
   - Mac: SpectraSuiteSetup_Mac.dmg
   - Linux: SpectraSuiteSetup_Linux

Downloading from the Ocean Optics ftp Site

Installing on a Windows Platform

Total download is approximately 30 MB.

► *Procedure*

1. Close all other applications running on the computer.
2. Type ftp://spectrasuite.oceanoptics.com into the browser.
3. Open FTP Site in Windows Explorer by clicking the Page menu and selecting **Open FTP site in Windows Explorer**.
4. Right-click on any white space in the browser window and select **Login As...**. The login and password dialog box appears.
5. Enter the following:

   Username: ***username***

   Password: ***password***
6. Double-click on **Installations**.
7. Drag SpectraSuiteSetup_Windows.exe to the local computer and execute. The default installation directory is **\Program Files\Ocean Optics\SpectraSuite**. The SpectraSuite icon location is **Start | Programs | Ocean Optics | SpectraSuite | SpectraSuite** and the current user's desktop.

Installing on a Macintosh Platform

You must be logged on as an administrative user to install SpectraSuite on your Mac. Total download is less than 15 MB.

► *Procedure*

1. Open a terminal window (Finder | Applications | Utilities | Terminal).
2. Type in your user name and password.
3. Paste the following text into this terminal window:

   ftp ftp://*username*:*password*@spectrasuite.oceanoptics.com
   hash 10000
   lcd ~/Desktop
   cd Installations
   get SpectraSuiteSetup_Mac.dmg
   quit

   When this command is finished, a file named **SpectraSuiteSetup_Mac.dmg** appears on the desktop.
4. Double-click on the SpectraSuiteSetup_Mac.dmg file to mount the disk image. A new SpectraSuite icon resembling a disk drive appears on your desktop. The new icon should open automatically (if it doesn't, double-click it).
5. Copy the SpectraSuite icon to your desktop.
6. When the installation is complete, drag the SpectraSuite drive icon to the recycle bin.

Installing on a Linux Platform

Total download is approximately 30 MB.

► *Procedure*

Open a terminal window.

1. Type in your user name and password.

   Paste the following text into the terminal window:ftp
   ftp://*username:password*@spectrasuite.oceanoptics.com
   hash 10000
   lcd ~/Desktop
   cd Installations
   get SpectraSuiteSetup_Linux.bin
   quit

   A SpectraSuiteSetup_Linux.bin file appears on your desktop.

2. Start a terminal window and enter the following commands:

   chmod 755 ~/Desktop/SpectraSuiteSetup_Linux.bin
   sudo ~/Desktop/SpectraSuiteSetup_Linux.bin

   You are prompted for your password, which allows you to execute the setup as root. Contact your system administrator if you do not have password.

   If the sudo command does not work (it may not be set up for your user account), then enter the following:

   su
   (enter password for root)
   ~/Desktop/SpectraSuiteSetup_Linux.bin

   The Linux version of SpectraSuite requires some libraries that may not be installed by default, depending on the Linux distribution. The following are libraries are required, and are not provided as part of SpectraSuite:

   - libstdc++ version 5. Some newer systems only install version 6, so a compatibility package may be required. In Fedora Core Linux, libstdc++ version 5 is provided by compat-libstdc++.
   - libXp version 6 (earlier versions may work too). In Fedora Core 3 and 4, this is provided in xorg-x11-deprecated-libs.
   - libusb version 0.1.10 or newer (should be provided in a libusb package or can be downloaded from http://libusb.sourceforge.net/download.html#stable).

   It may be necessary to modify SELinux (Security Enhanced Linux) restrictions before SpectraSuite will run. It is possible to remove SELinux auditing by running 'setenforce Permissive' as root or by customizing your SELinux policies. The SpectraSuite installer does not modify system security settings.

Note

The default installation directory is /usr/local/OceanOptics/SpectraSuite.

A symbolic link is put in /usr/bin so that you can enter **spectrasuite** on any command line to start the program.

The SpectraSuite icon ( ) location varies by installation, but will be under either Applications or Other under the Application Launcher menu.

Chapter 3

Controls and Indicators

Overview

SpectraSuite consists of a number of visual controls in the form of icons and buttons. This chapter describes these controls and how to use them.

Some menu selections and controls require that some action to be taken before they can be used. When unavailable, the controls are grayed-out. Many of these requirements will be lifted so that the software will ask what to do when it is not appropriate to take an action yet, but until then, the behavior is as follows:

Acquisition parameters, storing dark/reference spectra, and the Strip Chart require an unambiguous selection of an acquisition. If no acquisitions are running, try starting one. If more than one acquisition is started, try clicking on the desired trend in the graph to select the correct target. Similarly, try expanding the tree under the icon of the spectrometer and see how the controls respond to selecting each item. Right-click these items (or Control-click in MacOSX) to see additional actions for each.

Minus dark requires a dark spectrum to be stored.

A, T, R, and I (relative irradiance) require a dark and reference to be stored.

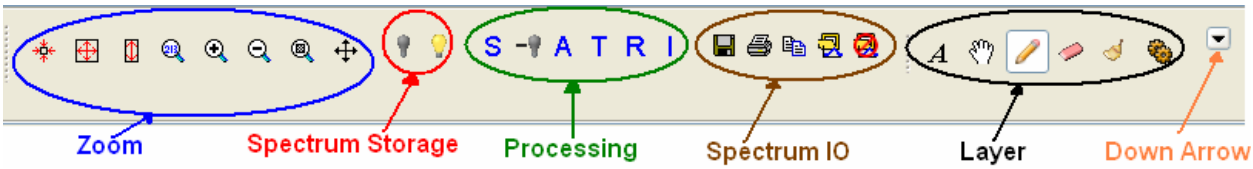
Absolute Irradiance mode (I) requires a calibration and a stored dark spectrum.

Photometry and energy/power/photons measurements require an active absolute irradiance calculation.

Graph Controls

The heart of the SpectraSuite application is the spectrum graph. SpectraSuite provides you with a wide variety of options to customize and monitor your graph views.

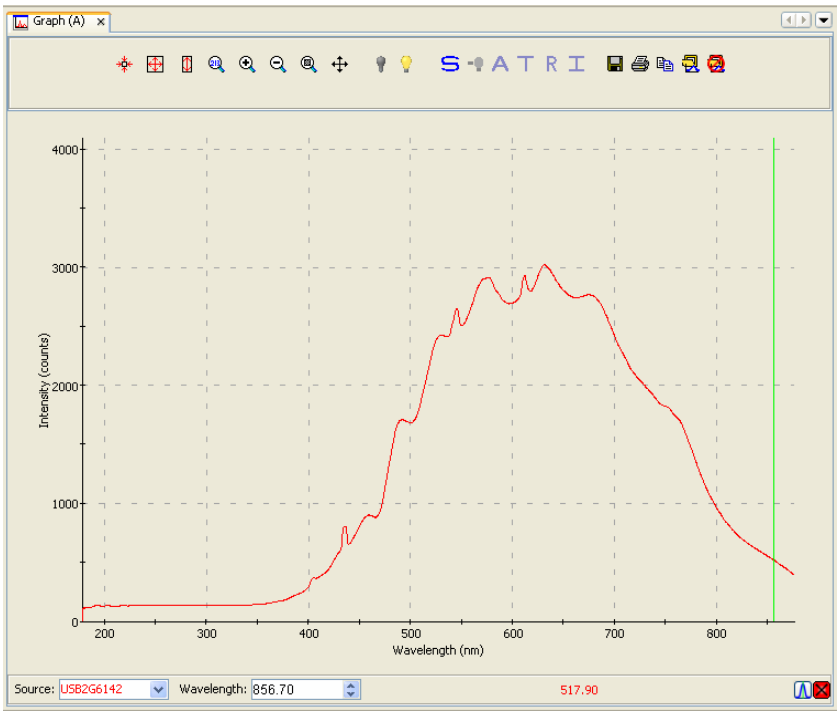
Controls are organized into the following toolbars that can be displayed or hidden using the Down Arrow button ( ).



Zoom Tools

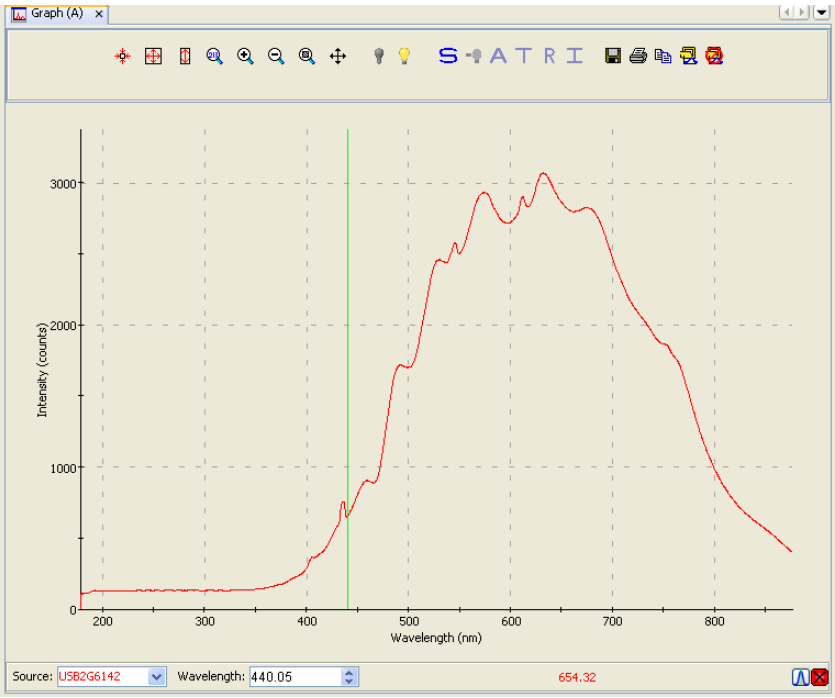
Zoom Out to Maximum

This control zooms out to display a full view of the spectrum graph.



Scale Graph to Fill Window

This control adjusts the graph display so that the section of the graph relevant to the spectrum line is shown, but no more. Both the x and y axis are adjusted. In this example, the graph is zoomed in so that the Y axis (Intensity) above 3500 no longer appears since the graph line does not extend that far.

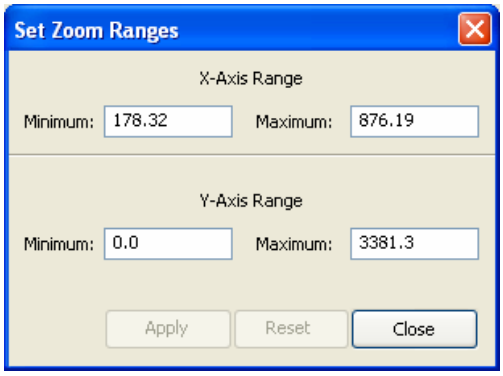


Scale Graph Height to Fill Window

Use this control to zoom in on a graph so that the full height of the spectrum line is shown, but no more. Unlike the Scale Graph to Fill Window control, only the y axis is adjusted.

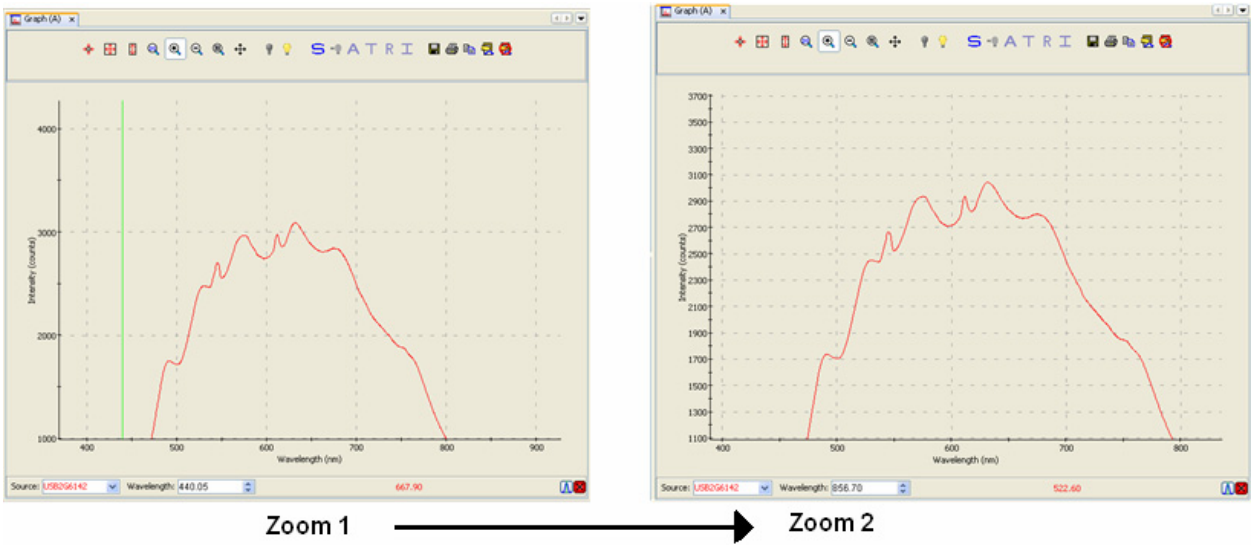
Manually Set Numeric Ranges

This control enables you to set the exact zoom coordinates. When you click on the control, the Set Zoom Ranges dialog box appears so that you can enter the desired coordinates.



Zoom In

Use this control to zoom in on the graph. Each time you click this control, the display zooms in further.



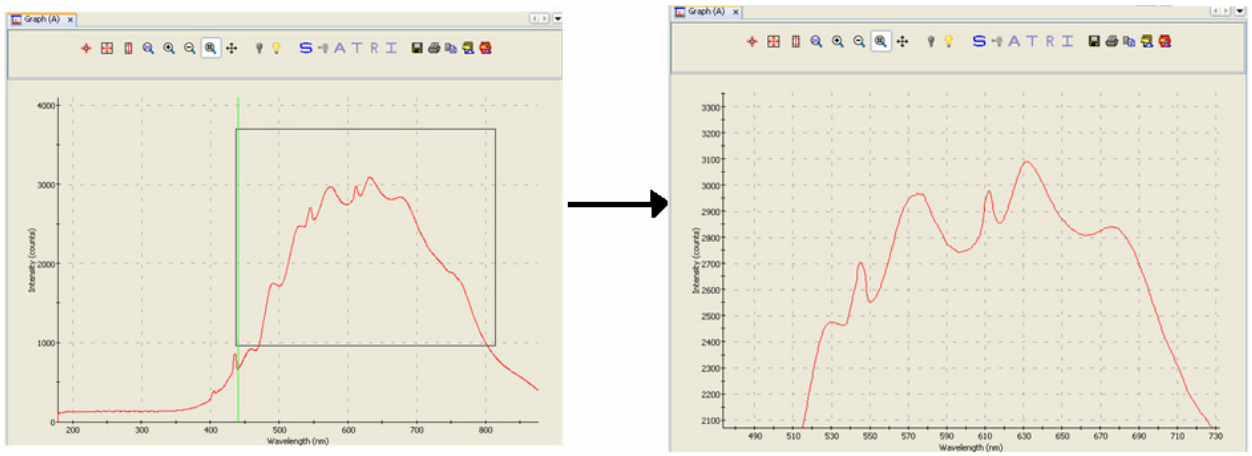
You can also use the mouse wheel to zoom in on the graph centered around the cursor (green vertical line).

Zoom Out

Use this control to reverse the zoom in process.

Zoom to Region

This control allows you to select a section of the graph to zoom in on. When you click the control, a cursor appears on the screen, enabling you to box-in a region to zoom in on.



Toggle Graph Pane

Use this control when you have more than one graph and want to switch between graph displays.

Spectrum Storage Tools

Icon	Meaning
	Store dark spectrum
	Store reference spectrum

These tools are also available from the **File | Store** menu. See *Store* for more information on these functions.

Processing Tools

Icon	Meaning
	Scope Mode
	Scope Minus Dark Mode
	Absorbance Mode
	Transmission Mode
	Reflection Mode
	Relative Irradiance Mode

These tools can also be accessed from the **Processing | Processing Mode** menu. See *Processing Mode* for more information on these functions.

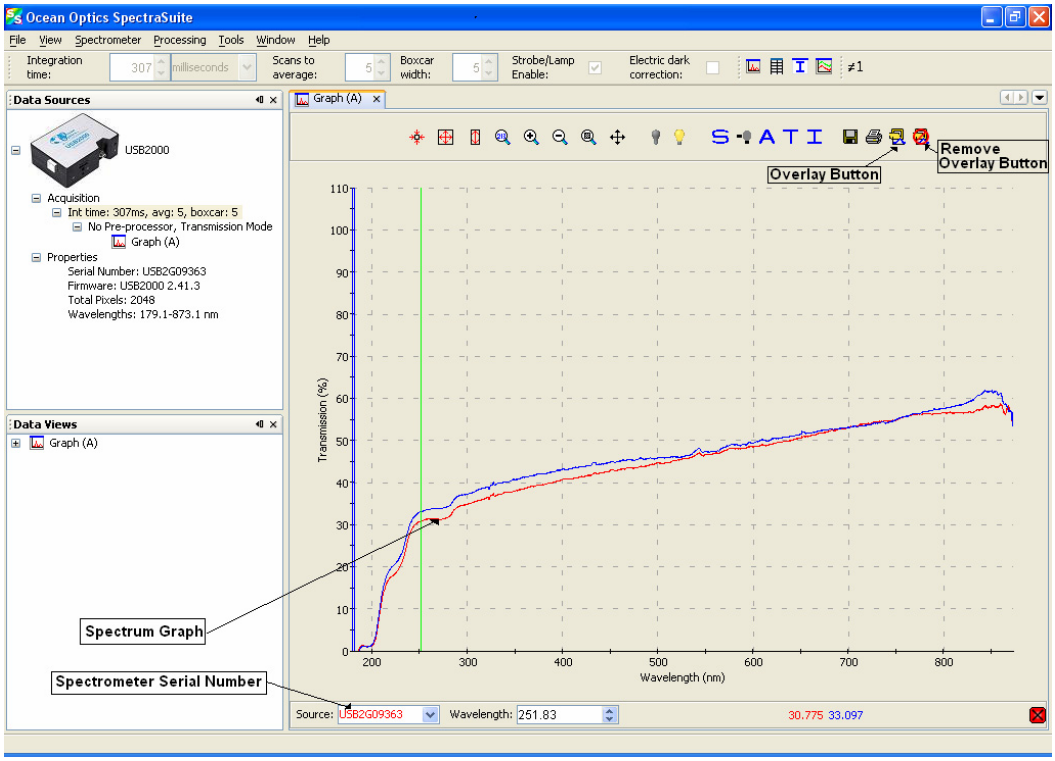
Spectrum IO Tools

Icon	Meaning
	Save Spectra. Click to save data in either a Grams SPC format, JCAMP format, binary format (which only SpectraSuite can read) or tab-delimited format (can be opened in an Excel spreadsheet).
	Opens the SpectraSuite Printing dialog box. Select what you want to print and to where (system printer, PDF file). You can select to print various layers on your graph, zoom in to a section of the graph, and add a title, if desired. You can adjust the font size and display of grid lines. The Preview button displays a view of how your printout will look.
	Copy spectral data to clipboard.

Icon	Meaning
	Overlay spectral data. Overlays a previously saved spectrum onto the current graph. See *Overlay Spectral Data* for more information.
	Delete overlay spectra. Deletes any spectra that have been overlaid on the current graph.

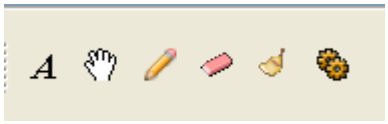
Overlay Spectral Data

The Overlay Spectral Data control enables you to display a saved spectrum on the current spectrum. Click this control, and then browse for the file that you want to overlay on the current graph. The overlay shows the spectrometer serial number and the filename that you loaded the overlay from.



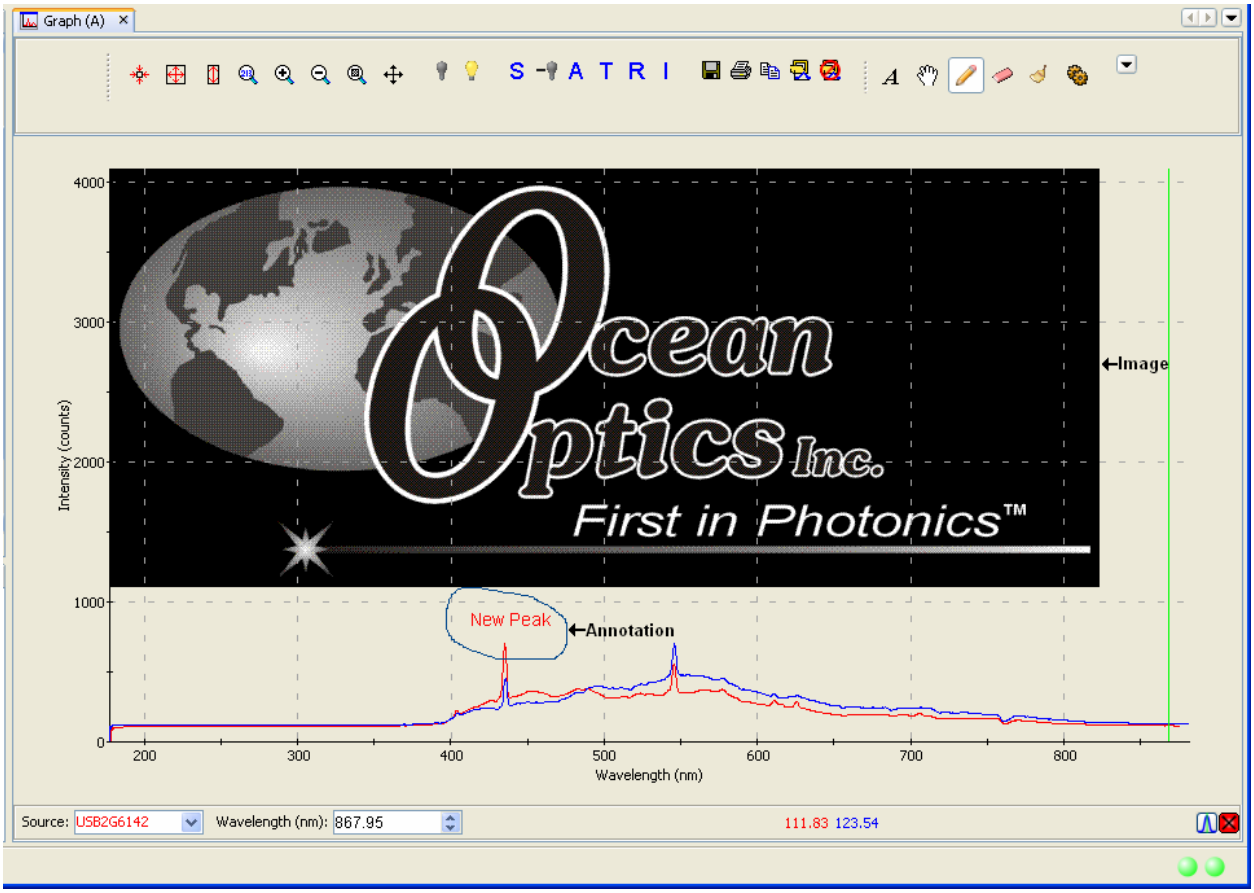
Layer Tools

The Layer tools provide you with functions to write captions and other meaningful data on your graphs. Select the tools using the Layer Toolbar.



Tool	Function
	Add New Annotation. Displays the New Annotation dialog box to add a new annotation to the selected graph.
	Select and Drag Annotation. Allows you to grab an annotation on the graph and drag it to another location.
	Draw. Allows you to draw freehand (using the mouse) on the graph.
	Erase Areas of Drawing Layer. Erases selected portions of the drawing created with the Draw tool (pencil).
	Clear Drawing Layer. Clears the entire drawing made with the Draw tool (pencil).
	Graph Layer Options. Displays the Graph Layer Options dialog box (see Graph Layer Options).

The following figure shows a graph with an image layer and an annotation circled with the drawing tool.



Other Controls

Acquisition Controls

Much like controls on a VCR, the Acquisition Controls allow you to pause and resume continuous spectra acquisition, and perform a single acquisition.

Control	Action
	Pause selected acquisition
	Perform single acquisition
	Resume selected acquisition

Peak Finding

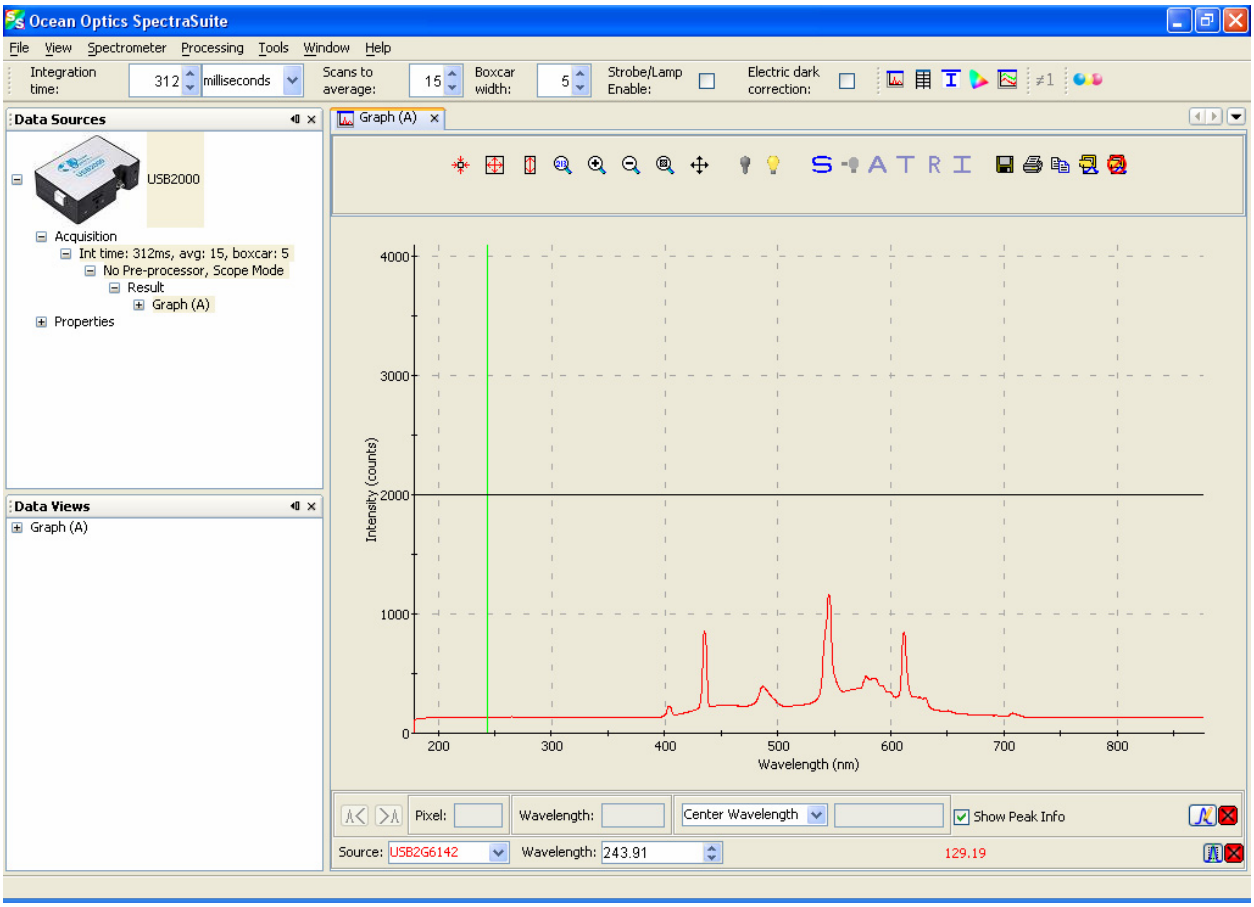
This control (located in the bottom, right corner of the graph) allows you to create a threshold on your spectral graph to isolate peaks.

Note

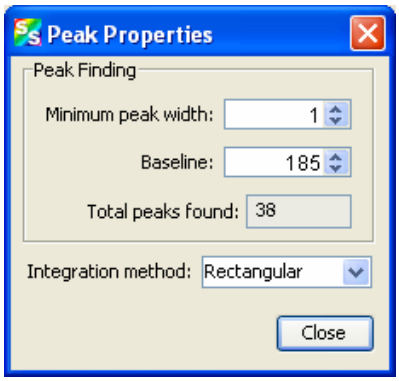
If this control does not display on your graph, click in the graph to make it appear.

► *Procedure*

1. Click . A threshold line appears on the graph, along with more Peak Finding controls. The threshold is set high and in most cases, should be adjusted.



2. Click to display the **Peak Properties** dialog box to set the threshold.



3. Set the threshold at the level needed to isolate the desired peaks. The threshold line moves into the location you selected.

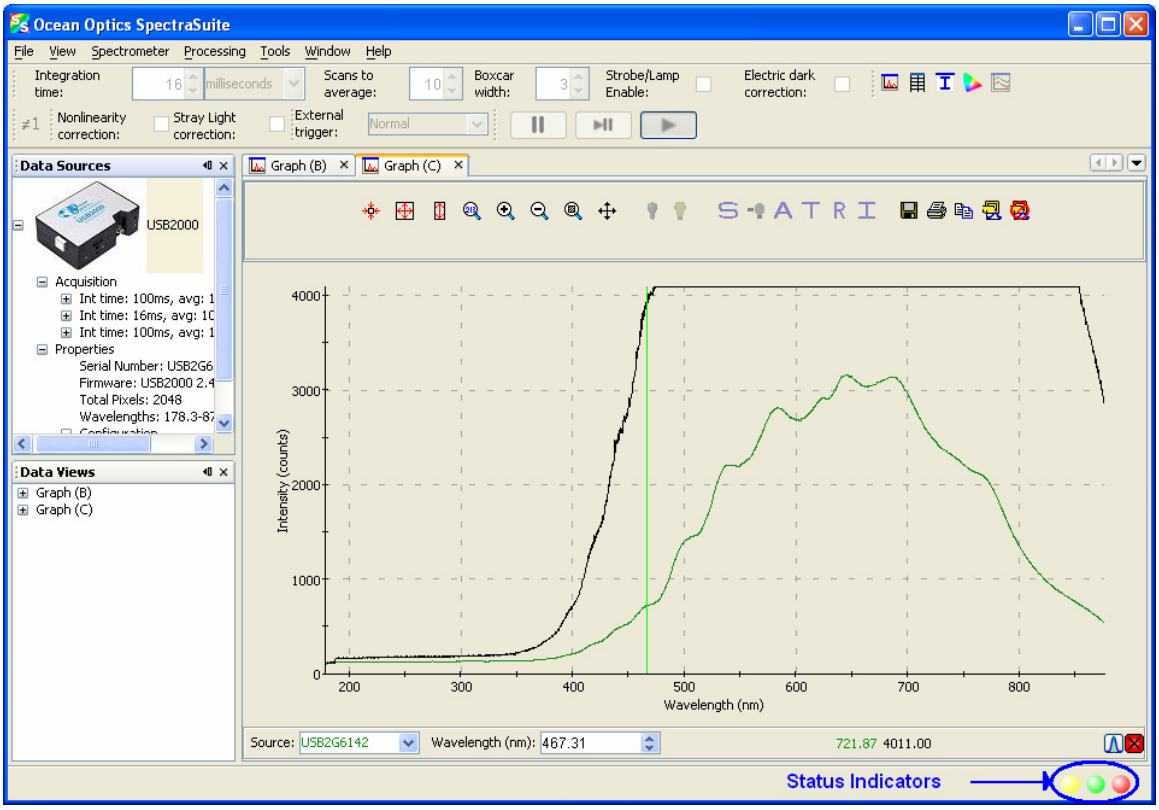
4. Use and to move the cursor to the next peak (left or right). The peak wavelength value appears in the **Wavelength** field below the graph.

5. Check **Show Peak Info** checkbox to display peak data in the Pixel and Wavelength boxes.

Indicators

Status

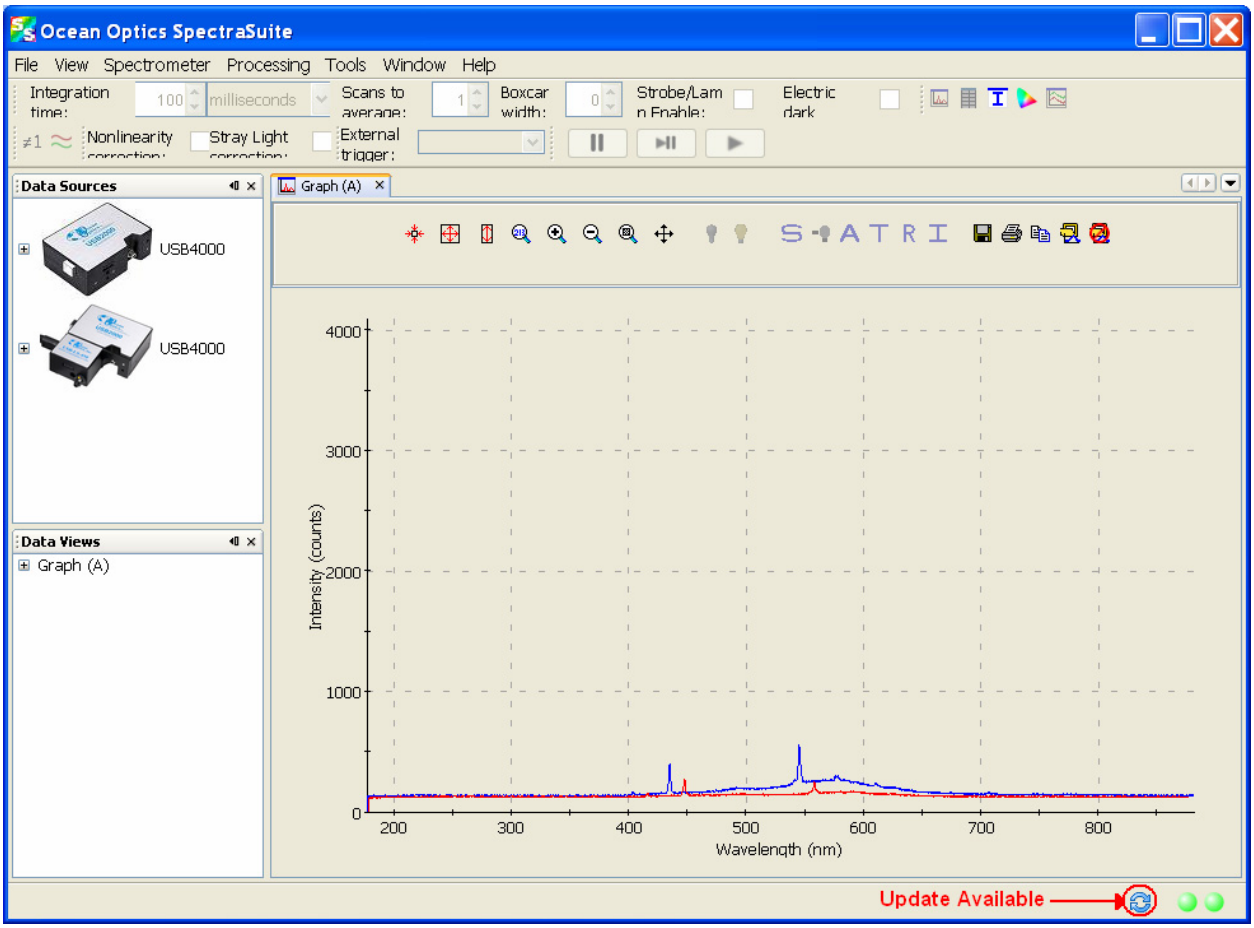
SpectraSuite provides you with feedback as to the status of the acquisitions you have graphed. The indicators refer to spectra shown on the graph currently displayed, as well as spectra on any other graphs that you have open (that appear on the graphs accessed from the tabs at the top of the screen). The feedback is in the bottom, right corner of the screen in the form of different colored circles. In the following example, two status indicators are shown for both spectral lines on Graph C, while a third indicator appears for the spectral line on Graph B.



Indicator	Meaning
	Recent acquisition within normal ranges
	Saturated signal
	Acquisition is paused
	Idle

Each circle corresponds to a graphed spectrum. If you pass the arrow pointer over a circle, it displays the spectrometer to which it refers and the related settings (e.g., **USB2G6142, Int time: 20 ms, avg: 10, boxcar: 3**). Click on a circle to select its associated spectrometer.

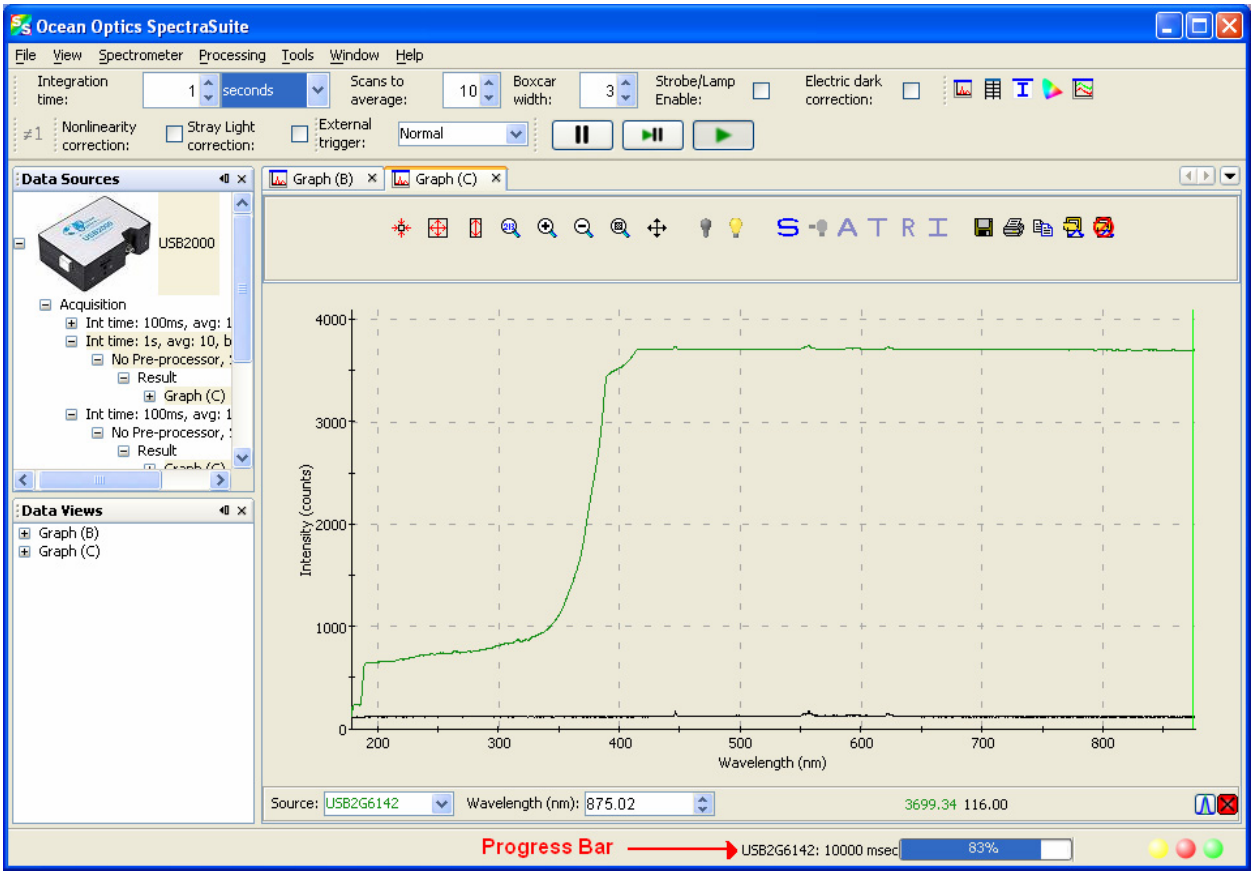
Update Available



Indicator	Meaning
	A software update is available to be downloaded. Go to **Tools | Update** center.

Progress Bar

If an acquisition takes longer than one second, a progress bar appears at the bottom of the screen. A progress bar can appear for each connected spectrometer that is acquiring data.



Chapter 4

File Menu Functions

Overview

This chapter details the various options and functions available from the File menu in SpectraSuite.

Where applicable, each section contains the associated toolbar icon below the section heading. Click on these icons in SpectraSuite to perform the described function.

New

The New menu selection displays the following list of functions that also are available from the Data Display toolbar:

Spectrum Graph

Spectrum Table

High-Speed Acquisition

Absorbance Measurement

Transmission Measurement

Reflection Measurement

Relative Irradiance Measurement

Gated Fluorescence Measurement

Curie Fluorescence Measurement

Gated Fluorescence Measurement

The New Gated Fluorescence Measurement menu selection is activated when you are using a spectrometer with a gated detector (such as the USB2000-FLG). When you select this menu item, a wizard leads you through the steps necessary to take a gated fluorescence measurement:

1. Selecting your source
2. Setting the data acquisition parameters
3. Taking a reference spectrum

4. Taking a dark spectrum
5. Setting your gated delay

See *Fluorescence* for more information on taking a fluorescence measurement.

Curie Fluorescence Measurement

The New Curie Fluorescence Measurement menu selection is activated when you are using a Curie UV-VIS Emission Spectrofluorometer (serial number starts with CUR).

Note

The Curie UV-VIS Emission Spectrofluorometer is a discontinued product.

When you select this menu item, a wizard leads you through the steps necessary to take a fluorescence measurement with a Curie spectrofluorometer.

Absolute Irradiance Graph

New Absolute Irradiance Measurement

New Concentration Measurement

Color Measurement

Strip Chart

Spectrum Graph

The Spectrum Graph menu option displays a new curve of spectral data on the open graph based on the parameters set in the Acquisition toolbar. Each new curve you create appears as a different color in the graph. Graphs appear in scope mode by default.

If you click on a curve, its corresponding parameters appear in the Acquisition toolbar. The data source (spectrometer) is listed in the Source box.

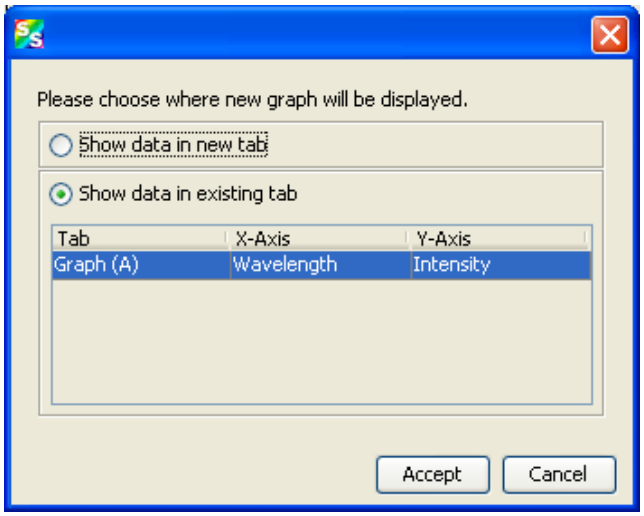
► *Procedure*

To display a spectral graph, follow the steps below:

1. Select **File | New | Spectrum Graph**

   Or

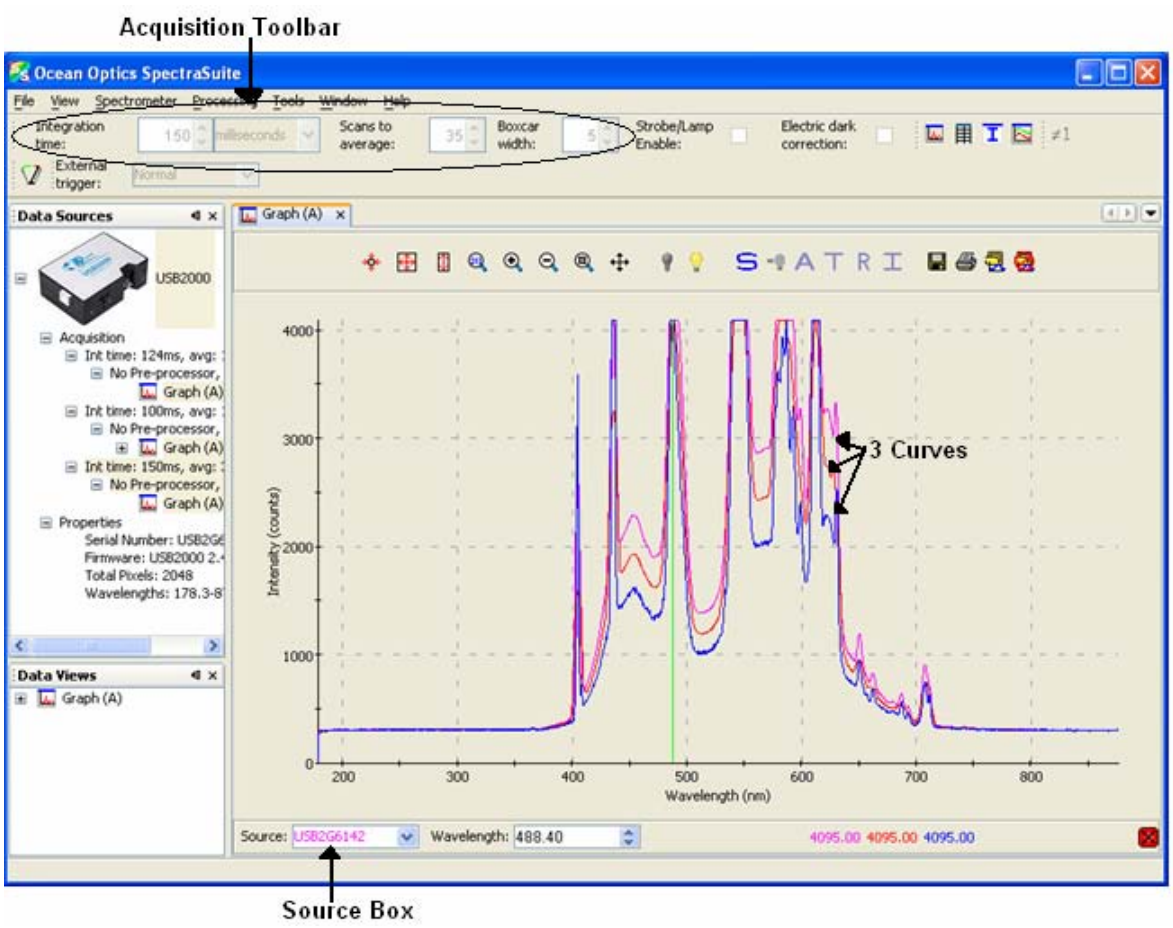
   Click in the Data Display toolbar. A dialog box appears asking if you want to display the new graph in the current graph tab, or start a new graph tab.



2. Choose where the new graph will be displayed and click Accept.

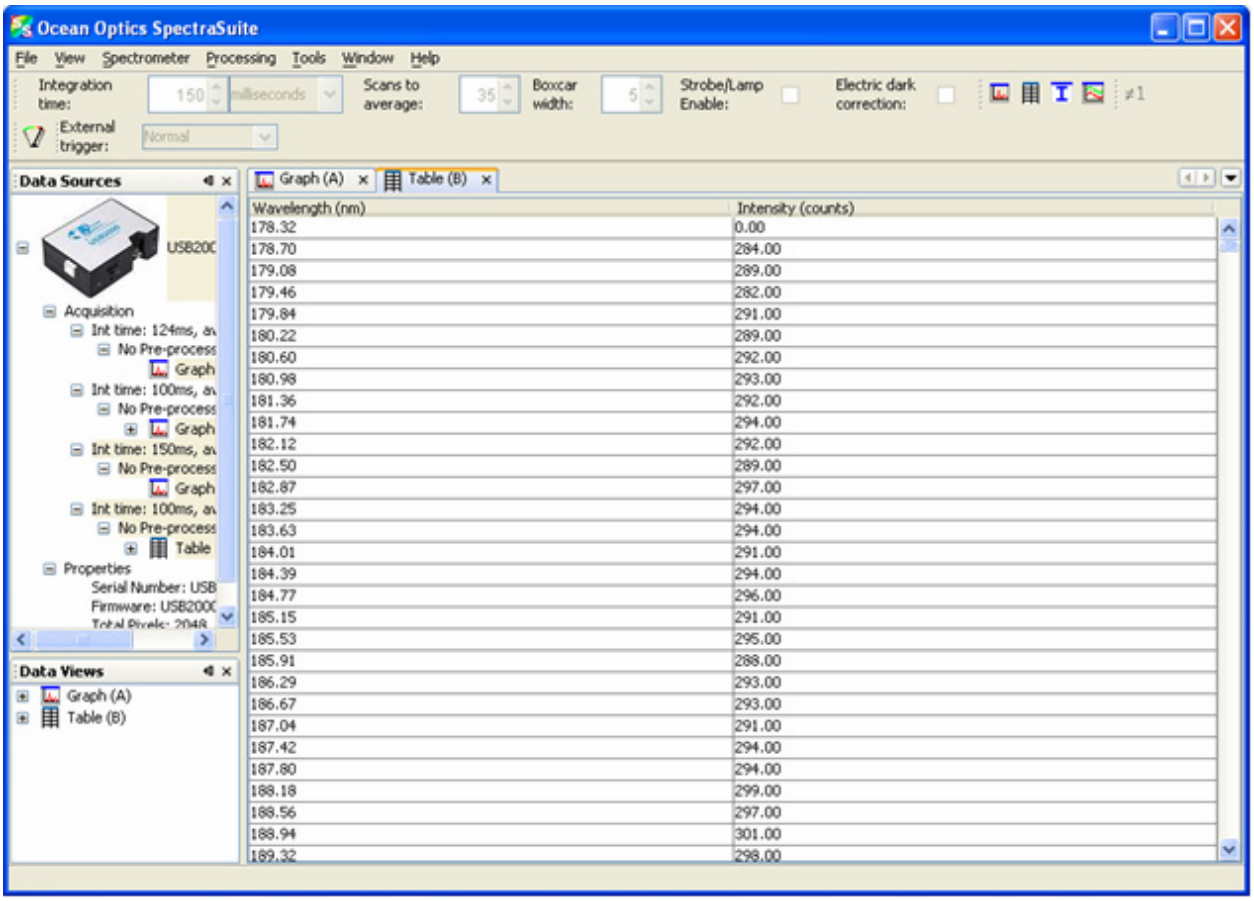
3. Set the desired parameters (integration time, scans to average, and boxcar width).

   The sample below shows a graph with three spectral curves (blue, pink and orange) in the same graph tab.



Spectrum Table

The Spectrum Table menu selection displays a spectral graph in tabular format. Select **File | Spectrum Table** from the menu or click in the Data Display toolbar. The spectrum table appears.



High-Speed Acquisition

Use this menu selection if you want to capture every scan at a very fast rate (20 ms or faster). SpectraSuite performs this high-speed data acquisition by capturing raw data without slowing it down by processing it. This captured high-speed data is called a spectra collection.

A spectra collection can be viewed in either a graph or table format. You can also record the captured data in a 3-dimensional graph, and then run other measurements on this captured data.

It's best to store your reference and dark spectra using the regular graph window before performing a high-speed data acquisition. The following procedure assumes that you do so.

High-Speed Data Capturing

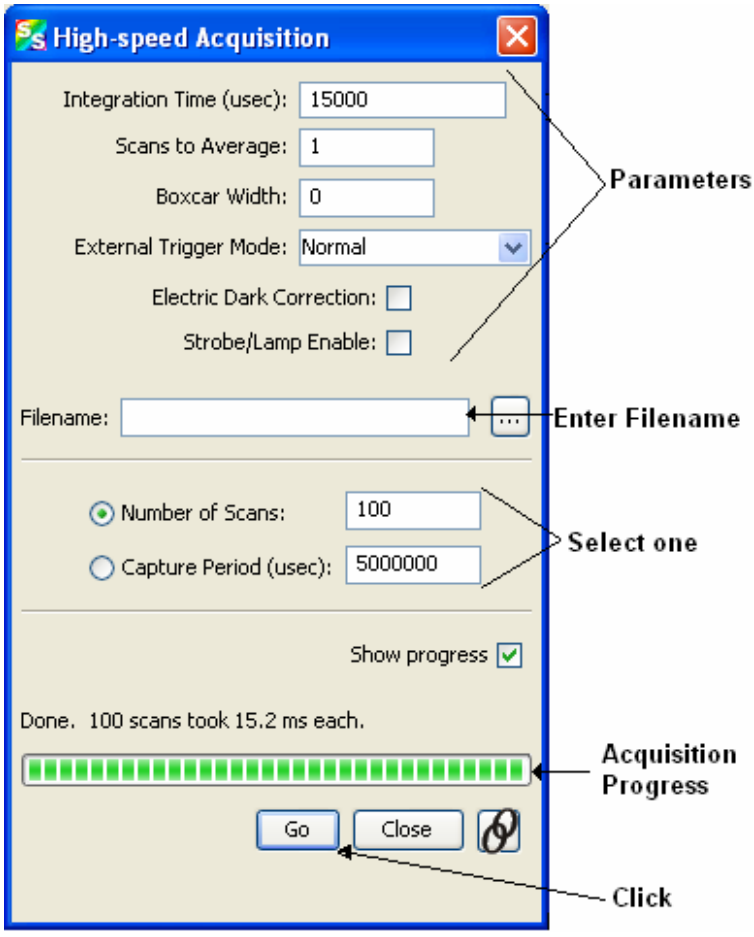
► *Procedure*

1. Save reference spectrum to a file. See *Reference*.
2. Save a dark spectrum to a file. See *Dark*.

Caution

To ensure accurate data, be sure that you have selected the same parameters (integration time, scans to average, and boxcar width) for your high-speed acquisition that you used when capturing your dark and reference spectra.

3. Select **File | New | High Speed Acquisition**. If you have other acquisitions running, a warning message appears telling you that all other acquisitions will be stopped when you are acquiring high speed data. Either stop all your other acquisitions, or click **OK** on this message and SpectraSuite will temporarily stop them. The **High-speed Acquisition** dialog box appears.



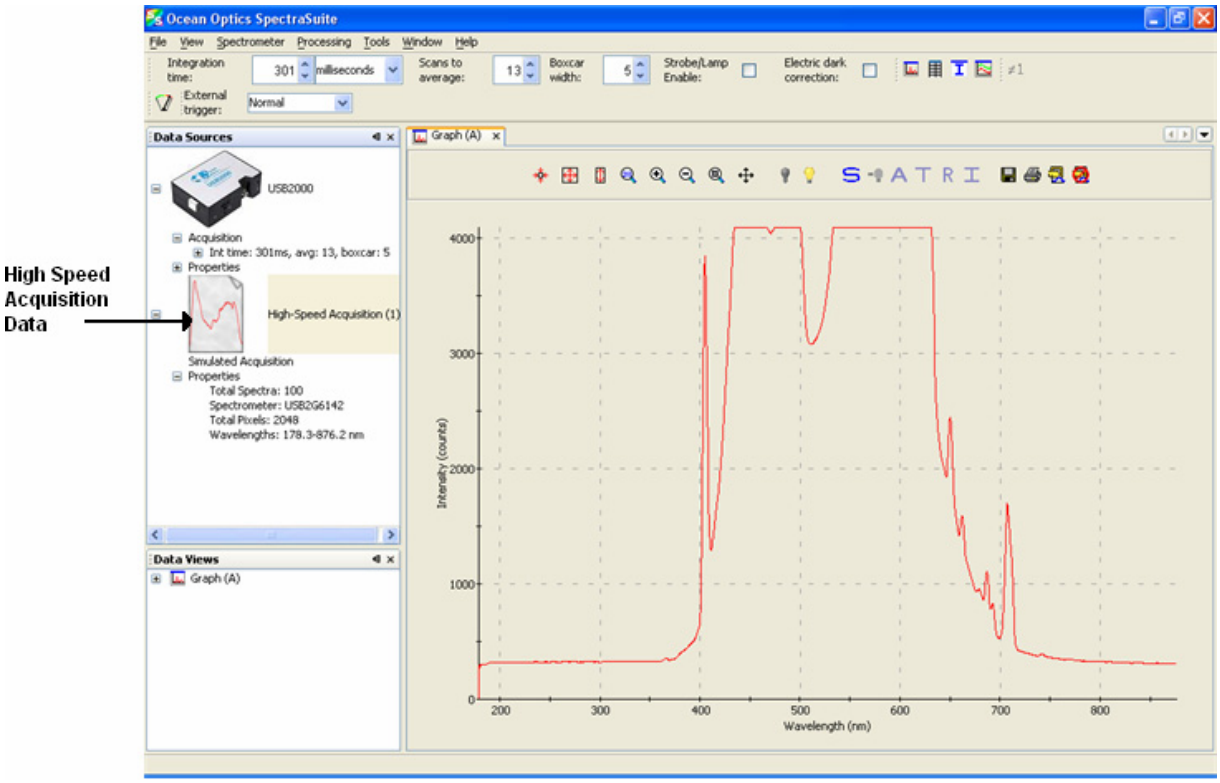
The top third of the form lists the parameters selected in the main graph window.

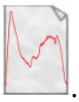
4. Enter the following information:

Field	Selection
Integration Time (µsec)	Specify the integration time in µsec.
Scans to Average	Enter the number of scans to average
Boxcar Width	Enter the boxcar width
External Trigger Mode	Select the external trigger mode (Normal, Software, Synchronization, External Hardware)
Electric Dark Correction	Enable this option for electric dark correction
Strobe/Lamp Enable	Enable this option to turn on the lamp
Filename	Enter the name or browse to the file where you want to store data in a tab-delimited format.
Number of Scans Or Capture Period (µsec)	Choose one of these methods of data acquisition Acquire a fixed number of scans (fastest method) Specify a time period for data capture
Show progress	Enable this option to show the progress of the acquisition.

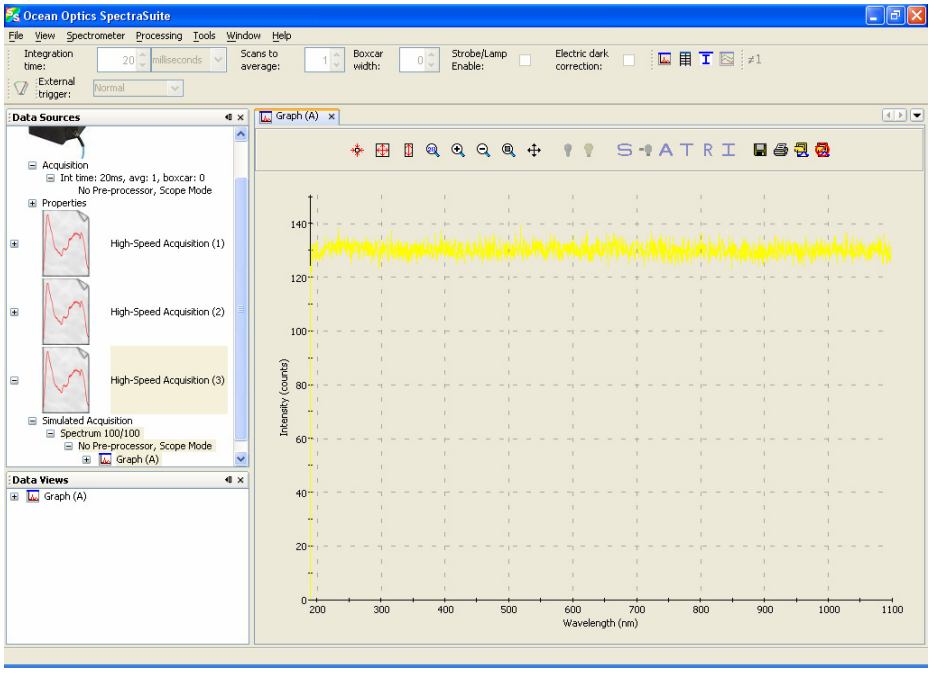
5. Click

. Your high-speed acquisition data appears in the **Data Sources** pane.



6. Right-click on  . A menu displays the following selections:

- **Spectrum Graph** – Displays a graph of the spectra



- **Spectrum Table** – Displays spectra data in a table format

Wavelength (nm)	Intensity (counts)	Wavelength (nm)	Intensity (counts)
178.32	0.00	178.32	0.00
178.70	283.00	178.70	288.00
179.08	282.00	179.08	289.00
179.46	284.00	179.46	283.00
179.84	282.00	179.84	287.00
180.22	286.00	180.22	288.00
180.60	288.00	180.60	287.00
180.98	294.00	180.98	289.00
181.36	293.00	181.36	292.00
181.74	291.00	181.74	294.00
182.12	289.00	182.12	291.00
182.50	291.00	182.50	293.00
182.87	294.00	182.87	292.00
183.25	289.00	183.25	289.00
183.63	292.00	183.63	292.00
184.01	296.00	184.01	293.00
184.39	295.00	184.39	295.00
184.77	291.00	184.77	292.00
185.15	293.00	185.15	294.00
185.53	293.00	185.53	292.00
185.91	292.00	185.91	293.00
186.29	297.00	186.29	287.00
186.67	288.00	186.67	292.00
187.04	294.00	187.04	292.00
187.42	293.00	187.42	290.00
187.80	295.00	187.80	291.00
188.18	295.00	188.18	289.00
188.56	293.00	188.56	293.00
188.94	287.00	188.94	294.00

- **Save Spectra Collection** – Stores the high-speed spectra in a file. See *Creating a 3-D Chart of High-Speed Acquisition Spectra* for more information about what can be done with stored high-speed spectra data.
- **Remove Spectra Collection** – Deletes the captured high-speed spectra collection data. You can also select **Spectrometer | Remove Spectra Collection**.

Creating a 3-D Chart of High-Speed Acquisition Spectra

You can create a 3-dimensional representation of the data over time in graph form. The navigation controls enable you to view the graph from different angles. Click on any point in the graph to display its value and wavelength.

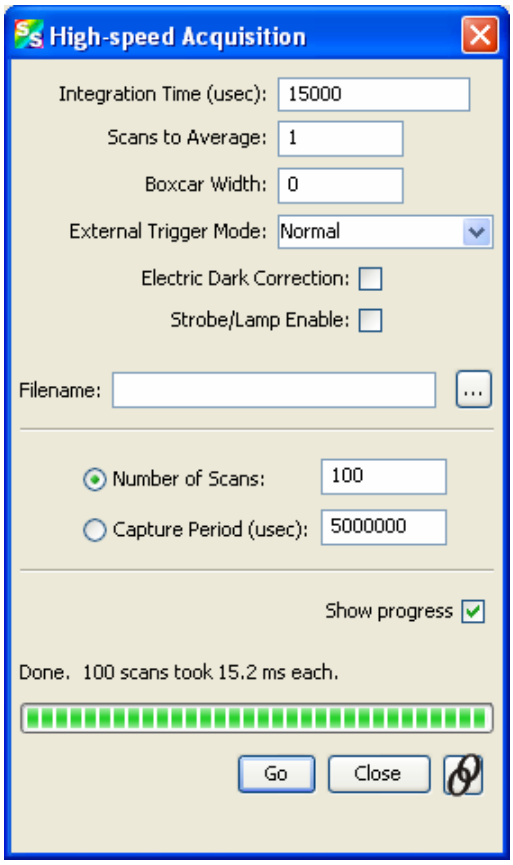
► *Procedure*

To create a 3-D graph,

1. Right-click on the spectrometer in the **Data Sources** pane and select **High Speed Acquisition**

   Or

   Select **File | New | High Speed Acquisition** from the menu. The **High-speed Acquisition** dialog box appears.



2. Enter the parameters and click . The 3-dimensional graph appears.

Using High-speed Acquisition Spectra

A spectra collection that you have stored using the high-speed acquisition feature has a variety of uses such as the following:

You can replay the spectra, fast forward, rewind, etc. just like any recorded data. Strip Chart data can also be replayed (see *Strip Chart* for more information on how to create a Strip Chart).

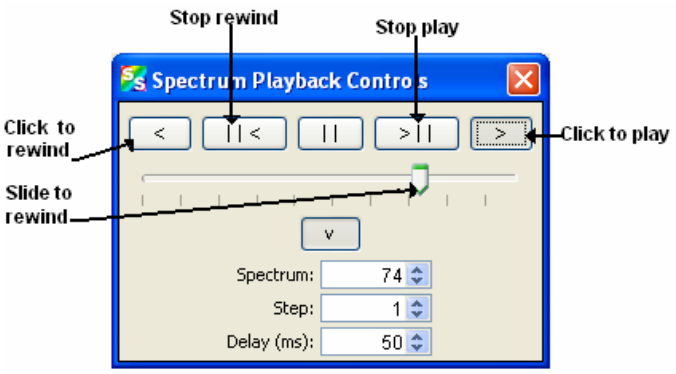
You can also conduct further experiments on the recorded data (absorbance, transmission, etc.) by clicking on the appropriate icon (**A**, **T**, **R**, or **I**).

► *Procedure*

To replay recorded data,

1. Right-click on the desired spectrum listed under **Simulated Acquisition** in the **Data Sources** pane. A menu appears.

2. Select **Spectrum Playback Controls**. The **Spectrum Playback Controls** dialog box appears.



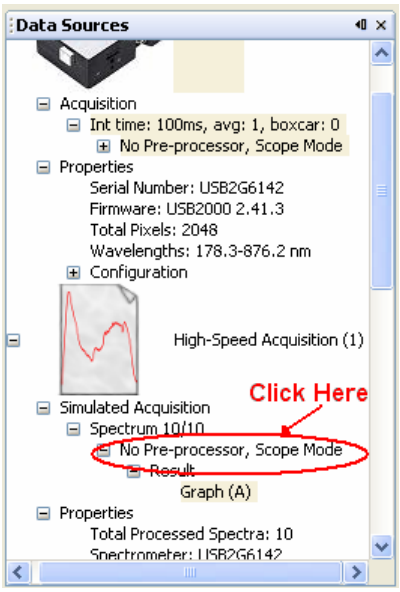
3. Rewind the recording, then press to play the recorded spectrum graph.

► *Procedure*

To do further processing on recorded data,

1. Begin playback of recorded data. Note that the tree in the **Data Sources** pane populates with the usual acquisition data.

2. If needed, load preprocessing data (dark and reference spectra) by right-clicking on **No pre-processor, Scope Mode** in the **Data Sources** pane and selecting **Load Reference Spectrum** and **Load Dark Spectrum**. Browse to the desired reference and dark files.



Or, you can store reference and dark spectra at any time during playback if you have the necessary data in your collection.

3. Once you have loaded the processed spectrum files, you can switch to another mode (Absorbance, Transmission, etc.) by clicking on the appropriate icon (, , etc.).

Absorbance Measurement

The Absorbance Measurement menu selection launches the Absorbance Measurement Wizard to facilitate taking an absorbance measurement using SpectraSuite. The wizard leads you through the steps necessary to take an absorbance measurement:

1. Selecting your source
2. Setting the data acquisition parameters
3. Taking a reference spectrum
4. Taking a dark spectrum

See *Absorbance Experiments* for more information on taking an absorbance measurement.

Transmission Measurement

The Transmission Measurement menu selection launches the Transmission Measurement wizard to help you through the process of taking a transmission measurement.

Reflection Measurement

The Reflection Measurement menu selection launches the Reflection Measurement wizard to help you through the process of taking a reflection measurement.

Relative Irradiance Measurement

The Relative Irradiance menu selection launches the Relative Irradiance Measurement wizard to help you take to help you through the process of taking a relative irradiance measurement.

Gated Fluorescence Measurement

The New Gated Fluorescence Measurement menu selection is activated when you are using a spectrometer with a gated detector (such as the USB2000-FLG). When you select this menu item, a wizard leads you through the steps necessary to take a gated fluorescence measurement:

1. Selecting your source
2. Setting the data acquisition parameters

3. Taking a reference spectrum
4. Taking a dark spectrum
5. Setting your gated delay

See *Fluorescence* for more information on taking a fluorescence measurement.

Curie Fluorescence Measurement

The New Curie Fluorescence Measurement menu selection is activated when you are using a Curie UV-VIS Emission Spectrofluorometer (serial number starts with CUR).

Note

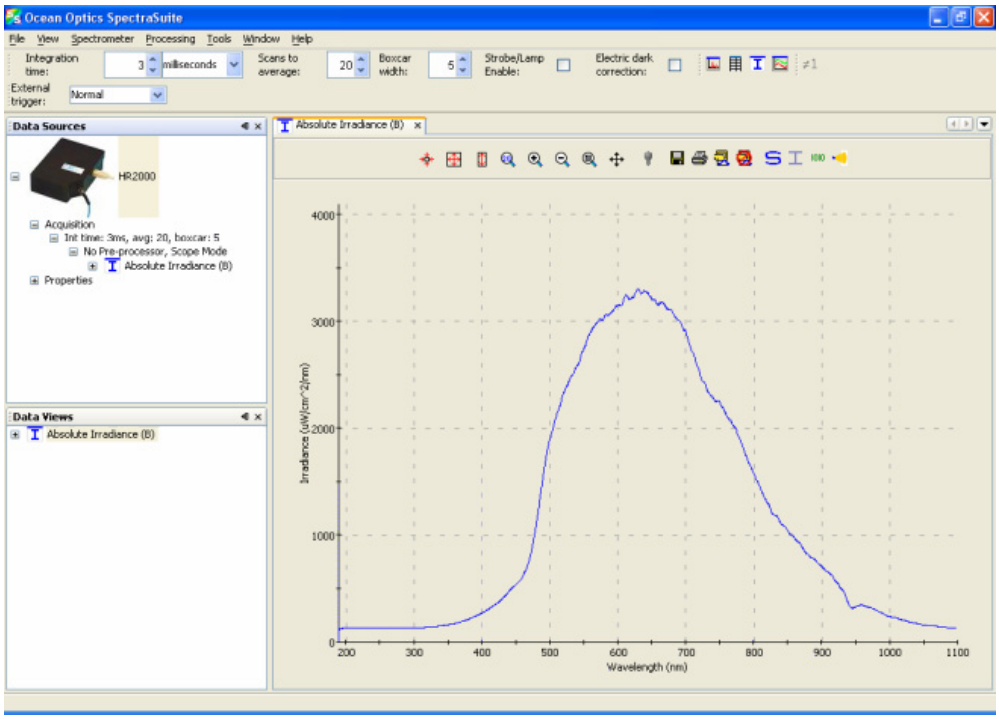
The Curie UV-VIS Emission Spectrofluorometer is a discontinued product.

When you select this menu item, a wizard leads you through the steps necessary to take a fluorescence measurement with a Curie spectrofluorometer.

Absolute Irradiance Graph

The Absolute Irradiance Graph menu selection displays the Absolute Irradiance graph. With SpectraSuite, you can display multiple spectra from multiple devices with independent calibrations. You can also calculate integrated intensities (watts, joules, photons) and photometric quantities (lux, lumen, candela).

Select **File | Absolute Irradiance Graph** from the menu. The Absolute Irradiance Graph in Scope mode appears. See *Absolute Irradiance in Appendix A: Experiment Tutorials* for more information.



New Absolute Irradiance Measurement

The New Absolute Irradiance Measurement menu selection launches the Absolute Irradiance Wizard to facilitate taking an absolute irradiance measurement using SpectraSuite. The wizard leads you through the steps necessary to take an absolute irradiance measurement:

1. Selecting your source
2. Setting the data acquisition parameters
3. Taking a reference spectrum
4. Taking a dark spectrum
5. Calibrating the spectrometer

See *Absolute Irradiance* for more information on taking an absolute irradiance measurement.

New Concentration Measurement

Concentration is the amount of a specified substance in a solution. Graphs of absorbance vs. concentration are known as Beer's Law plots. These are prepared by measuring the light absorbed by a series of solutions with different *known* concentrations. The length of the sample, such as the path length of our cuvette holder, and the wavelength chosen for monitoring the amount of light absorbed are constants. A linear plot from taking scans of these standard solutions with known concentrations is then obtained. The plot is then used to determine the *unknown* concentrations of substances in solutions.

Color Measurement

With SpectraSuite, you can calculate and report the Color Rendering Index (CRI) and Correlated Color Temperature (CCT) for your samples. SpectraSuite will compute all color measurements except RGB. You can only perform color measurements on one spectrometer at a time.

Emissive color measurements – Require a spectrometer, which has been calibrated to take irradiance readings (either relative or absolute). SpectraSuite gives you the option of choosing to measure either emissive or reflective color from either absolute or relative irradiance.

Reflective color measurements – Do not require an irradiance calibration, but they do require a reference spectrum. This reference scan is taken with the same optical configuration, except a perfect reflector is placed at the same location as the samples.

Strip Chart

SpectraSuite allows you to use Strip Charts to track processes, perform kinetic analyses, and monitor spectral events all as a function of time. The Strip Chart shows you how the value that you selected appears over time. This value can be any of the following:

One pixel (a single wavelength)

The average of a range of pixels

An integral calculated by one of three methods representing the area beneath the graph's trend line

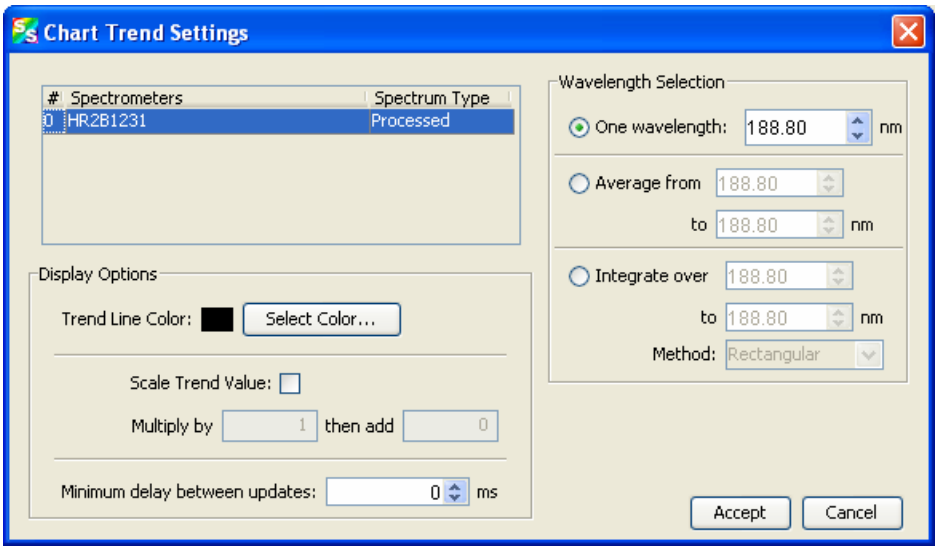
You can acquire this data using any processing mode (transmission, absorbance, etc.).

► *Procedure*

1. Place SpectraSuite in Scope mode by clicking the Scope ( ) icon in the Experiment mode toolbar or selecting **Processing | Processing Mode | Scope** from the menu.
2. Store a reference spectra and dark spectra.
3. Choose the measurement mode (absorbance, transmission, etc.).
4. Click the Strip Chart button ( )

   OR

   Select **File | New | Strip Chart** from the menu. The **Chart Trend Settings** dialog box opens.



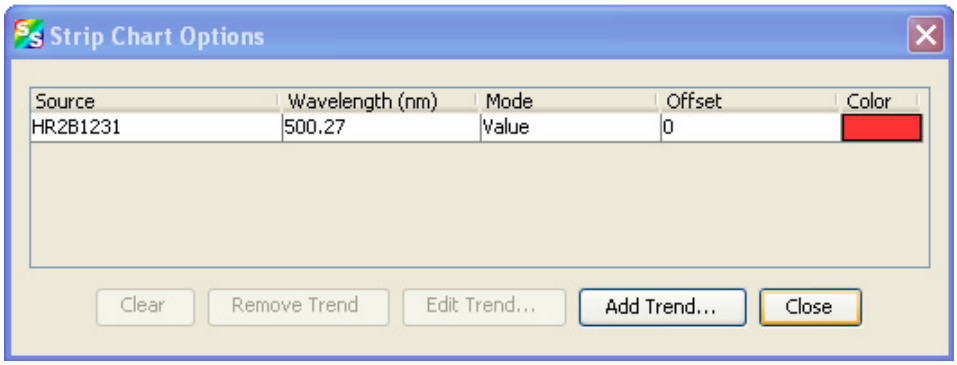
5. Enter the following data to create your Strip Chart:

Field	Selections
Wavelength Selection	Select the type of data for which you want to view the time trend. Select from the following: One wavelength – For one pixel (used in fluorescence, for example). Select the wavelength. Average from – For a range of pixels. Select the starting and ending wavelengths. Integrate over – For the area underneath the trend line. Select the starting and ending wavelengths. Then, select the method for calculating the continuous area underneath the graph curve: Rectangular, Simpson's, or Trapezoid.
Display Options	Select a color for the graph's trend line.
Scale Trend Value	If you would like to adjust your data, enter the appropriate information in this field.
Minimum delay between updates	Set the amount of time (in milliseconds) between data points on the graph. This delay is independent of the integration time. The data appears at the slower rate. **NOTE:** The longer the time between updates, the less computer memory that is used.

6. Click Accept. The Strip Chart Options dialog box appears. Strip Chart Options lists all of the Strip Charts that you have created, along with the options that you have set for each one. Use this dialog box to add, edit, remove, or clear trends.

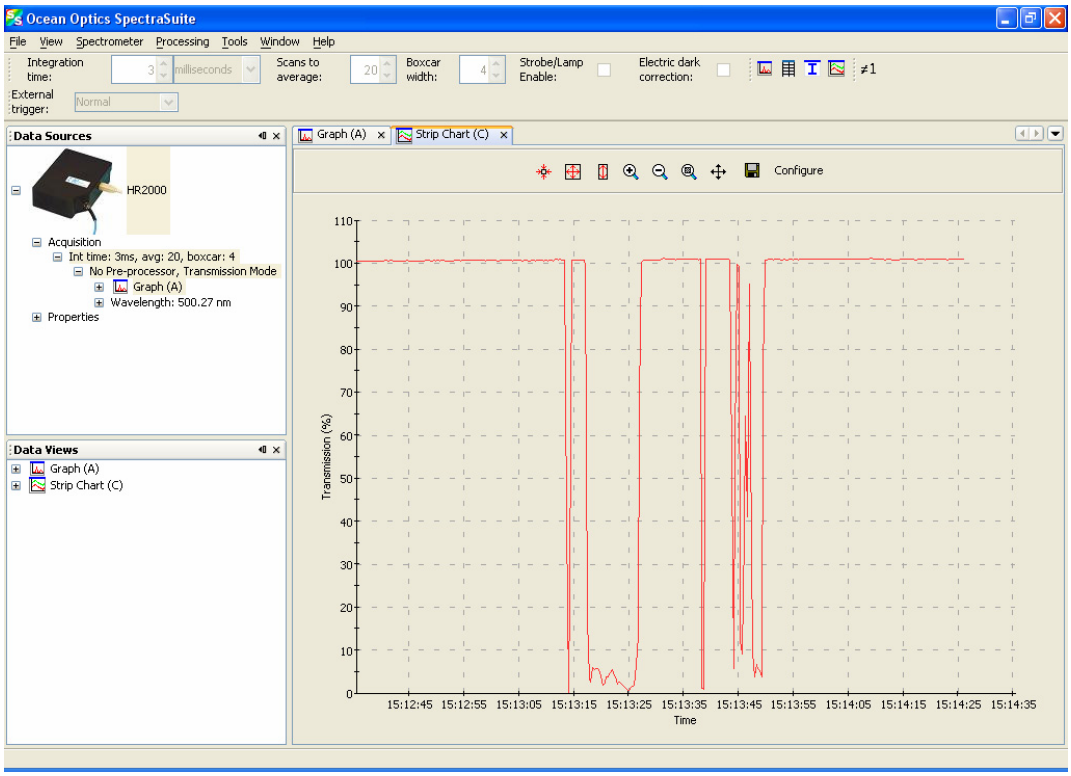
Note

Highlight the desired trend to make the **Clear**, **Remove Trend**, and **Edit Trend** buttons active.



7. Click Accept. The strip chart you created appears. Note the time scale along the x-axis. The y-axis in this example shows the percentage transmission for the selected pixel(s).

8. To add another trend to this graph, click Add Trend....



Open

Selecting the **Open** menu option allows you to load previously stored dark spectra, reference spectra, processed spectra, or all stored all spectra files. Select the type of spectrum to load, then browse to where the file is stored.

Dark

A dark spectrum is a spectrum taken with the light path blocked.

Select **File | Open | Load Dark Spectrum** to select and open one or more dark spectra.

Reference

A reference spectrum is a spectrum taken with the light source on and a blank in the sampling region.

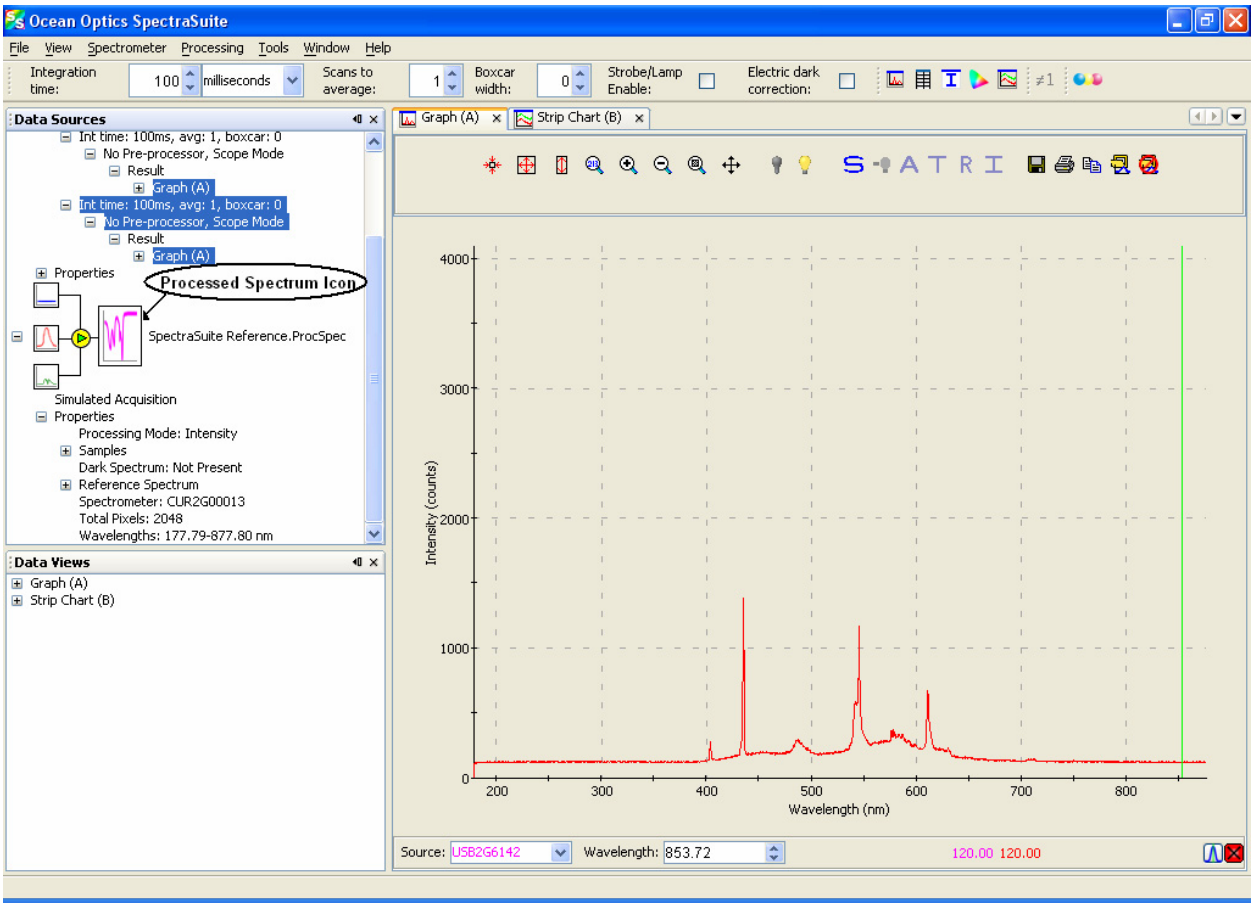
Select **File | Open | Load Reference Spectrum** to select and load one or more reference spectra.

Processed Spectrum

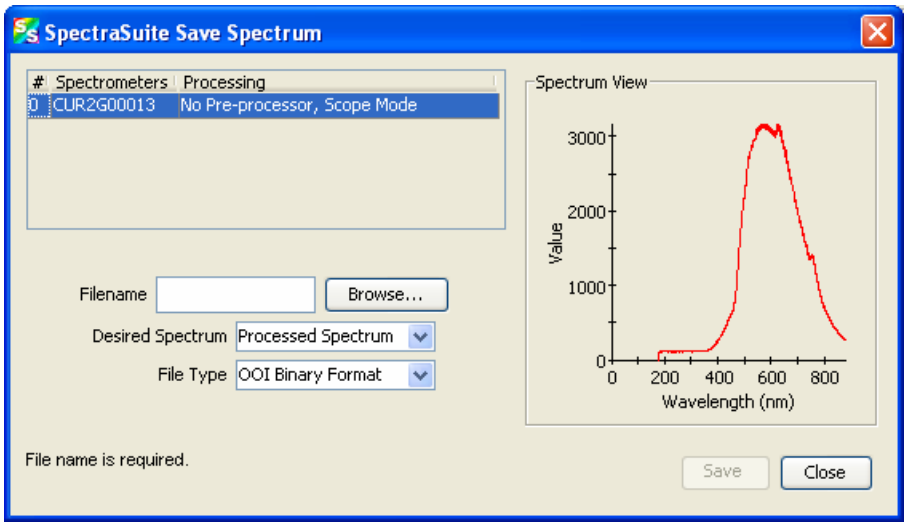
You have the ability to load a previously stored processed spectrum file.

► *Procedure*

1. Select **File | Open | Load Processed Spectrum** from the menu.
2. Type the file name or browse to the location of the desired processed spectrum file and open the file. The Processed Spectrum icon appears in the **Data Sources** pane.



3. You can save this processed spectrum back out to a file as processed, reference or dark spectrum. Right-click on the Processed Spectrum icon to display the SpectraSuite Save Spectrum dialog box.



4. Enter the file name or browse to a desired file, select the desired spectrum (processed, reference or dark), and select the file type (binary or tab-delimited).

Tip

Save the file as tab-delimited if you want to display it in an Excel spreadsheet.

5. Click Save....

Spectrum Collection

A spectrum collection is created when you perform a high-speed acquisition. Select **File | Open | Load Spectrum Collection** to browse to and open a spectrum collection from a high-speed acquisition.

Save

Save Spectra Collection

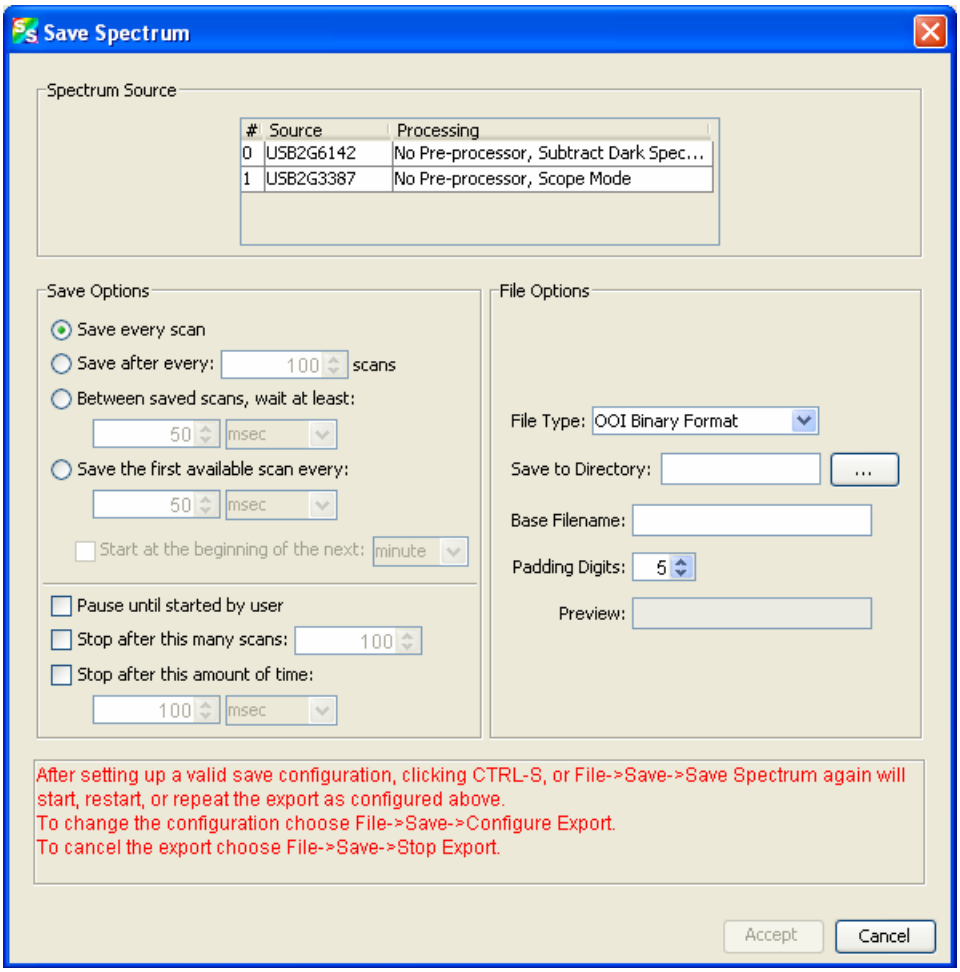
This menu option allows you to save your spectra collection to a file. Select **File | Save | Save Spectra Collection** from the menu and enter a file name. Also see *Exporting Processed Data* for information on exporting data to a file.

Save Spectrum

This menu options displays the Save Spectrum dialog box. Use this box to configure how you want to save your spectra. After you set the options and click Accept, choosing **File | Save | Save Spectrum** or typing CTRL + S exports the spectrum according to your settings in this dialog box.

To change these settings, select **File | Save | Configure Export**.

To cancel the export of the spectra, select **File | Save | Stop Export**.


Save Spectrum
Spectrum Source
Source Processing
0 USB2G6142 No Pre-processor, Subtract Dark Spec...
1 USB2G3387 No Pre-processor, Scope Mode
Save Options
Save every scan
Save after every: 100 scans
Between saved scans, wait at least:
50 msec
Save the first available scan every:
50 msec
Start at the beginning of the next: minute
Pause until started by user
Stop after this many scans: 100
Stop after this amount of time:
100 msec
File Options
File Type: OOI Binary Format
Save to Directory:
...
Base Filename:
Padding Digits: 5
Preview:
After setting up a valid save configuration, clicking CTRL-S, or File->Save->Save Spectrum again will start, restart, or repeat the export as configured above.
To change the configuration choose File->Save->Configure Export.
To cancel the export choose File->Save->Stop Export.
Accept
Cancel

Store

Use this menu selection to store reference and dark spectra before running your experiment.

Dark

A dark spectrum is a spectrum taken with the light path blocked.

Select **File | Store | Store Dark Spectrum** from the menu to save a dark spectrum to a file. You can also click in the graph toolbar.

Reference

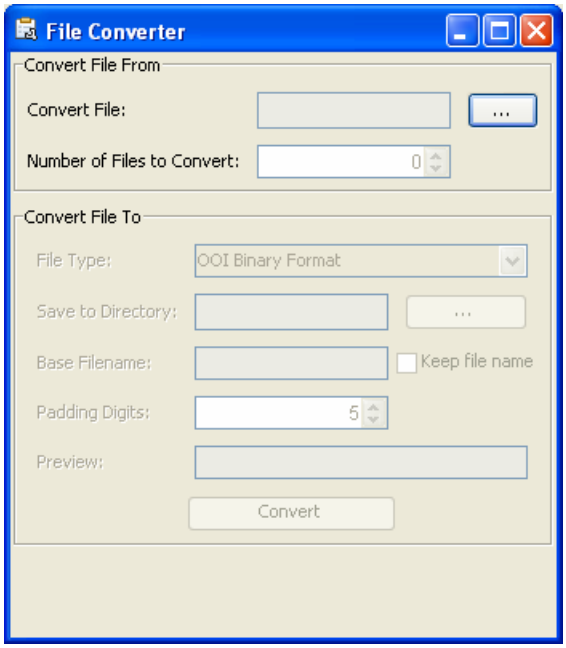
A reference spectrum is a spectrum taken with the light source on and a blank in the sampling region.

Select **File | Store | Store Reference Spectrum** to store a reference spectrum file. You can also click in the graph toolbar.

Convert Spectra

This function enables you to convert between file types.

Select **File | Convert Spectra**. The **File Converter** dialog box appears. Use this dialog box to select the file(s) to convert and to specify the file type desired.

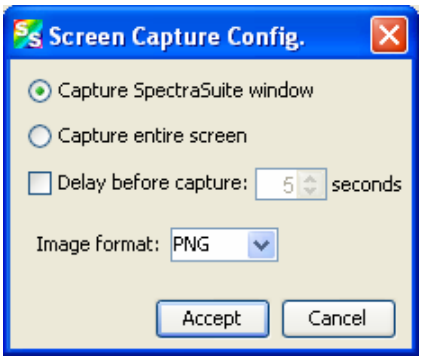


Screen Capture

This function takes a snapshot of the current SpectraSuite window, or the entire computer screen and stores it in the format and location that you specify.

► *Procedure*

1. Select **File | Screen Capture**. The **Screen Capture Config.** dialog box appears.



2. Select to capture either the just SpectraSuite window or the entire computer screen.
3. If you don't want to capture the screen immediately, set a delay time.
4. Select to store the captured image as a PNG or JPG file.
5. Click Accept.
6. You are prompted to choose a name and location to store the captured file, then click Save.

Exit

Caution

For Mac operating systems, do NOT attempt to exit from the SpectraSuite application by using Quit. If you do so, the application could hang. Should this occur, unplug, then replug in the spectrometer(s) before restarting SpectraSuite to make the application work again.

Select **File | Exit** from the menu to exit the SpectraSuite application. A shutdown confirmation dialog box appears. Click **Yes** to exit SpectraSuite.

Alternately, you can click the top right **X** box of the application's display window.

Note

If your system gets hung after requesting SpectraSuite to shut down, press the Escape key twice to exit the application.

Chapter 5

View Menu Functions

Overview

This section details the various options and functions available from the **View** menu in SpectraSuite.

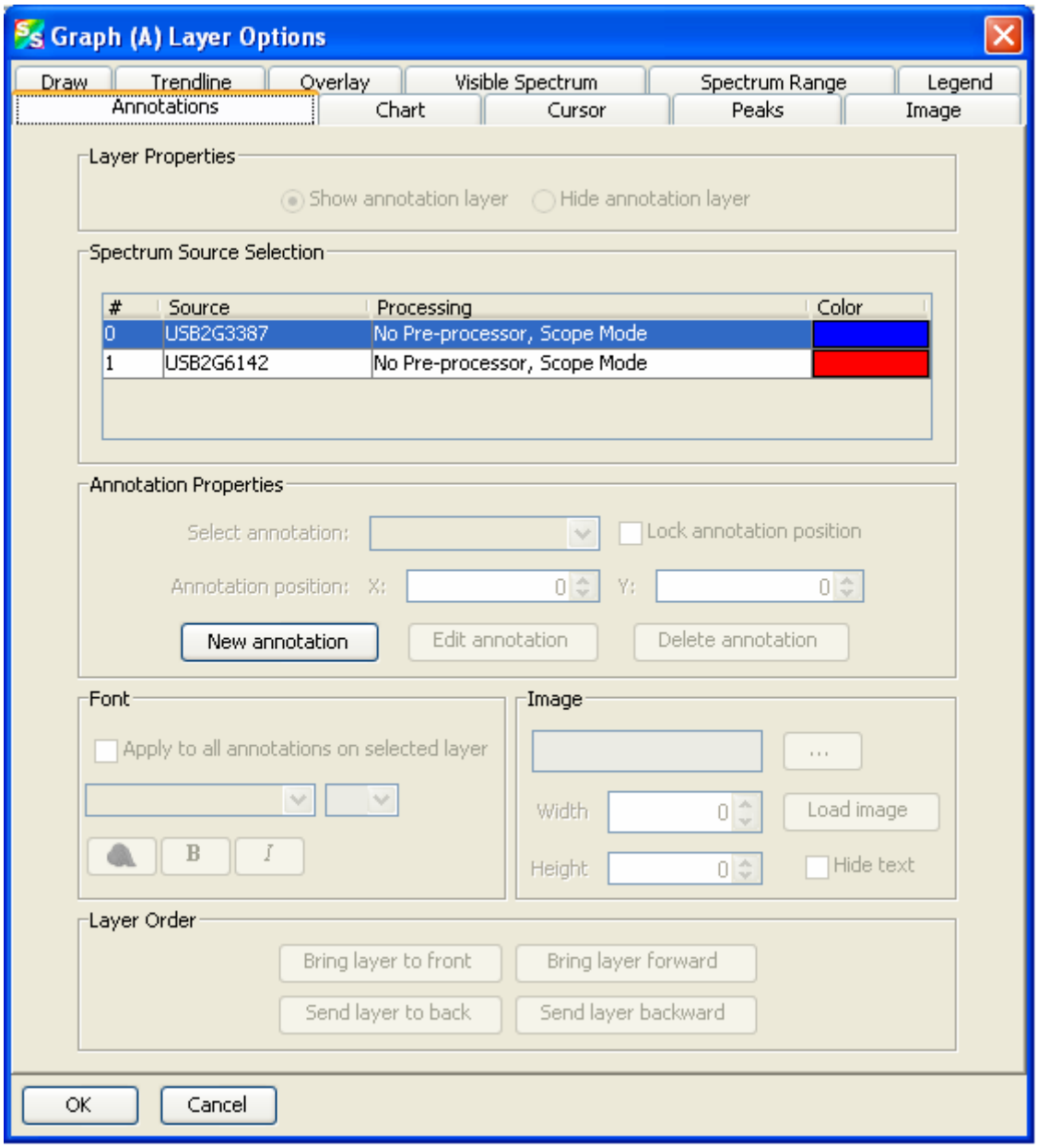
Scale

Empty

This menu selection is for future use.

Graph Layer Options

Select **View | Graph Layer Options**, right-click on the graph and select **Graph Layer Options**, click , or type CTRL+ALT+L to display the Graph Layer Options dialog box. The Graph Layers feature provides more control over the customization of your graph window.



Annotations

The Annotations functionality allows you to add text or an image to a specific location on the graph. Annotations are associated with a specific source (selectable by you), and when the source is removed, the annotations associated with it are removed as well. A subset of this functionality is also available by right-clicking on the graph or clicking (to add an annotation).

Chart

Use Chart to modify the following chart settings on the graph:

Chart line pattern

Chart line width

Font size

Chart background

Number precision for x and y axes

Number spacing for x and y axes

Tick spacing for x and y axes

Grid spacing for x and y axes

Grid lines

Grid line color

Cursor

Use the Cursor tab to modify the cursor color.

Peaks

Peaks functionality enables you to perform the following peak monitoring actions:

Display values on the graph relating to the peak such as peak value, center wavelength, pixel number, centroid, etc.

Set an alarm when a peak is reached. You can pause the acquisition, save the spectrum, and sound a customizable alarm.

Image

This option allows you to add a background image to your graph. You can set the size and orientation of the image, as well as flipping, rotating, stretching and skewing it. You can also lock the image in place for a given unit range.

Draw

Provides tools for modifying the appearance of the line created by the drawing tool ( ).

Trendline

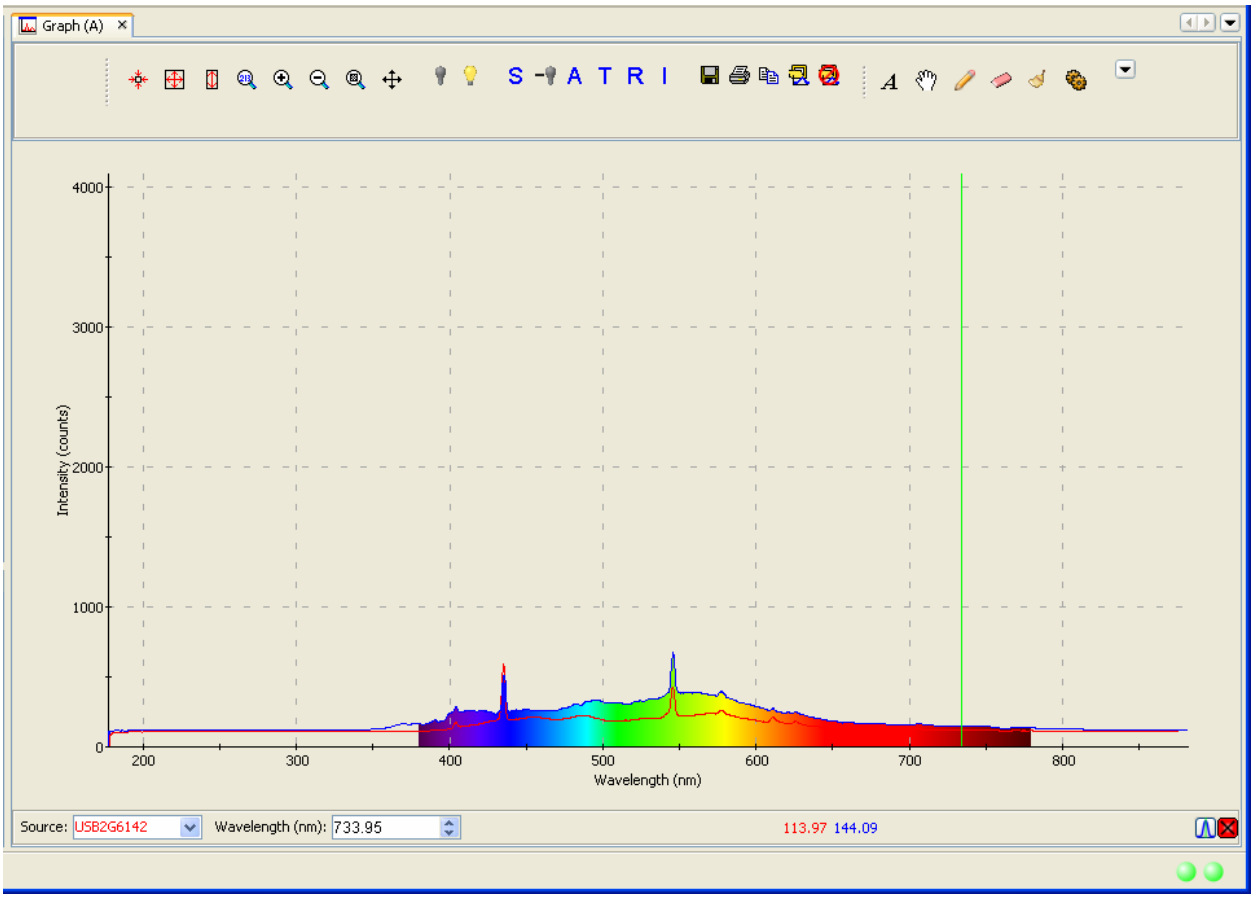
This option enables you to change the color and width of the trend line for the selected graph.

Overlay

Use this function to add an overlay to the selected graph.

Visible Spectrum

This option allows you to display the visible spectrum on your graph. You can display the spectrum the full height of the chart, as a bar on the x-axis, or beneath the selected trend line (as shown in figure below).

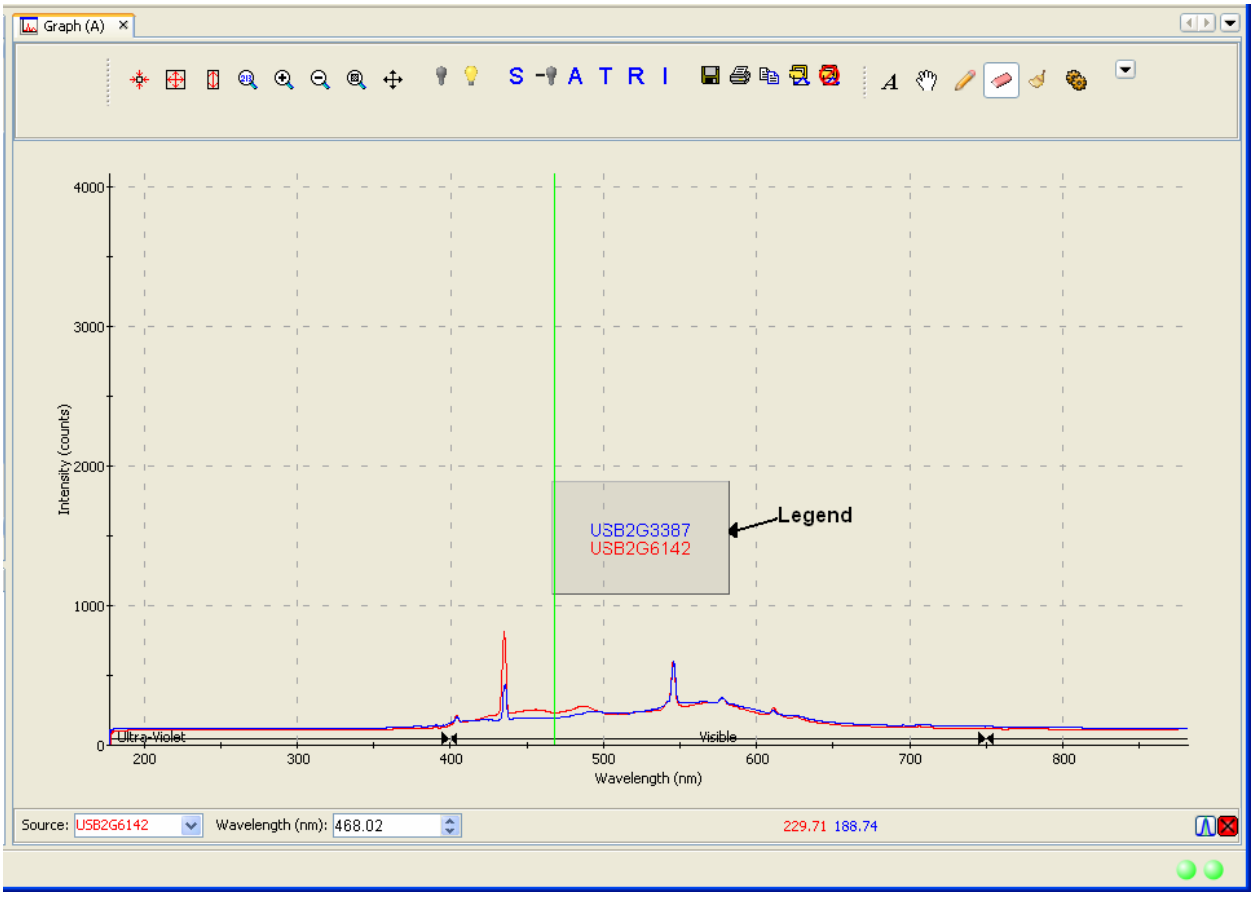


Spectrum Range

Spectrum Range allows you to display captions for the following spectrum ranges: Gamma, X-ray, UV, Visible, Near infrared, Mid infrared, Far infrared, Microwaves, and Radiowaves.

Legend

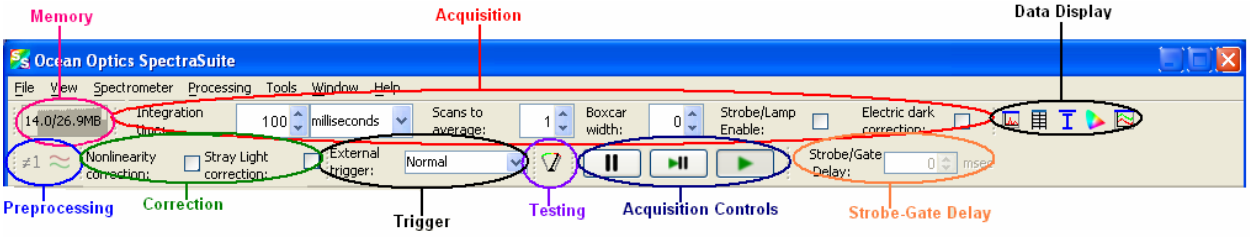
Use this option to add a customizable legend to your graph. The legend shows the spectrometer serial number and the name of the file that you loaded the overlay from, if applicable.



Toolbars

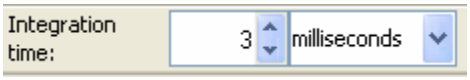
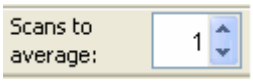
This menu item controls which toolbars are visible on the SpectraSuite window. Click on the following selections to toggle the toolbar on and off. When a toolbar is visible, a checkmark appears next to the menu selection.

The toolbars available from this menu item are shown on the SpectraSuite window in the figure below:



Acquisition

Select **View | Acquisition** to display/hide the tools related to the data being acquired and displayed in SpectraSuite.

Tool	Function
	Specifies the integration time of the spectrometer, which is analogous to the shutter speed of a camera. The higher the integration time, the longer the detector monitors the incoming photons. If your Scope mode intensity is too low, increase this value. If the intensity is too high, decrease this value. Adjust the integration time so that the greatest amount of light that you anticipate for your application causes a signal of about 85% of spectrometer's capability (for example, 3500 for spectrometers with a total of 4096 counts, 14000 counts for spectrometers with a total of 16384 counts, 50000 for spectrometers with a total of 65535 counts). While watching the graph trace, adjust the integration time until the signal intensity level is appropriate for the device. The integration time specified controls enabled spectrometer channels in the active spectral window.
	Specifies the number of discrete spectral acquisitions that the device driver accumulates before SpectraSuite receives a spectrum. The higher the value, the better the signal-to-noise ratio (S:N). The S:N will improve by the square root of the number of scans averaged.
	Sets the boxcar smoothing width, a technique that averages across spectral data. This technique averages a group of adjacent detector elements. A value of 5, for example, averages each data point with 5 points to its left and 5 points to its right. The greater this value, the smoother the data and the higher the signal-to-noise ratio. If the value entered is too high, a loss in spectral resolution will result. The S:N will improve by the square root of the number of pixels averaged.

Tool	Function
	Enables or disables the spectrometer strobe control function. This function toggles the S0 line of the spectrometer.
	Enables or disables the correction of the spectral data for electrical dark signal. For example, if the first 24 pixels in the spectrometer, while producing an electrical signal, do not respond to light then this option subtracts the average value of these first 24 pixels from the entire spectrum.

Acquisition Controls

Select **View | Toolbars | AcquisitionControls** to display/hide the tools for pausing and resuming continuous spectra acquisition. A control is also available for performing a single acquisition.

Control	Action
	Pause selected acquisition
	Perform single acquisition
	Resume selected acquisition

Correction

This toolbar has one tool: the nonlinearity correction checkbox. This tool enables/disables the detector linearity feature. The Correction toolbar only displays when you select it with **View | Toolbars | Correction**; it is absent from the screen by default.

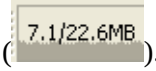
Data Display

The Data Display toolbar contains the icons for the following graph functions:

Icon	Function
	Spectrum Graph. Displays a new spectrum curve on the current graph with the parameters selected in the Acquisition toolbar. Each spectrum curve appears on the graph in a different color. The Acquisition parameters for each curve are listed in the Data Sources pane.

Icon	Function
	Spectrum Table. Displays the data acquisition in a table format. A tab for the table appears at the top pf the graph pane. See *Spectrum Table* for more information.
	Absolute Irradiance Graph. Displays a graph of absolute irradiance data. This graph appears on its own page with a tab at the top of the graph pane. It is also listed in the **Data Views** section.
	Color Measurement. Launches the Color Measurement wizard. See *Color Measurement* for more information.
	Strip Chart. Allows you to track processes, perform kinetic analyses, and monitor spectral events all as a function of time. See *Strip Charts* for more information.

Memory

The Memory toolbar consists of a display of the memory being used by the SpectraSuite application (

). Click this icon to force SpectraSuite to clean unneeded data from memory. The Memory toolbar only appears when you select it with **View | Toolbars | Memory**; it is absent from the screen by default.

Preprocessing

The Preprocessing toolbar contains icons for the following functions:

Icon	Function
	Nonunity correction. Performs a calculation to compensate for a reflection standard that is not perfectly white.
	Add Reference Monitor. Adjusts the signal to compensate for variations in spectral intensity based on light source and system drift.

SeaChanger

This control ( ) enables you to adjust the SeaChanger Color Engine(s) connected to a CDS LanBox-LCE, via Ethernet cable. You must have a Red Tide (USB650) spectrometer with an attached light source to use this SpectraSuite function.

► ***Procedure***

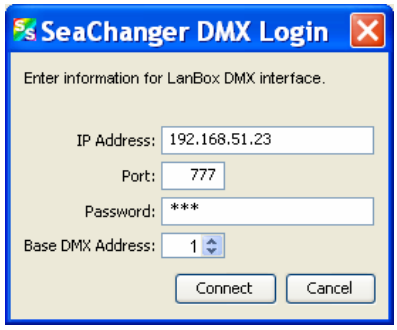
1. Click the SeaChanger control ( ) in the toolbar. The **Choose DMX Source** dialog box appears.

2. Select **None** or **LanBox DMX** for your source, then click

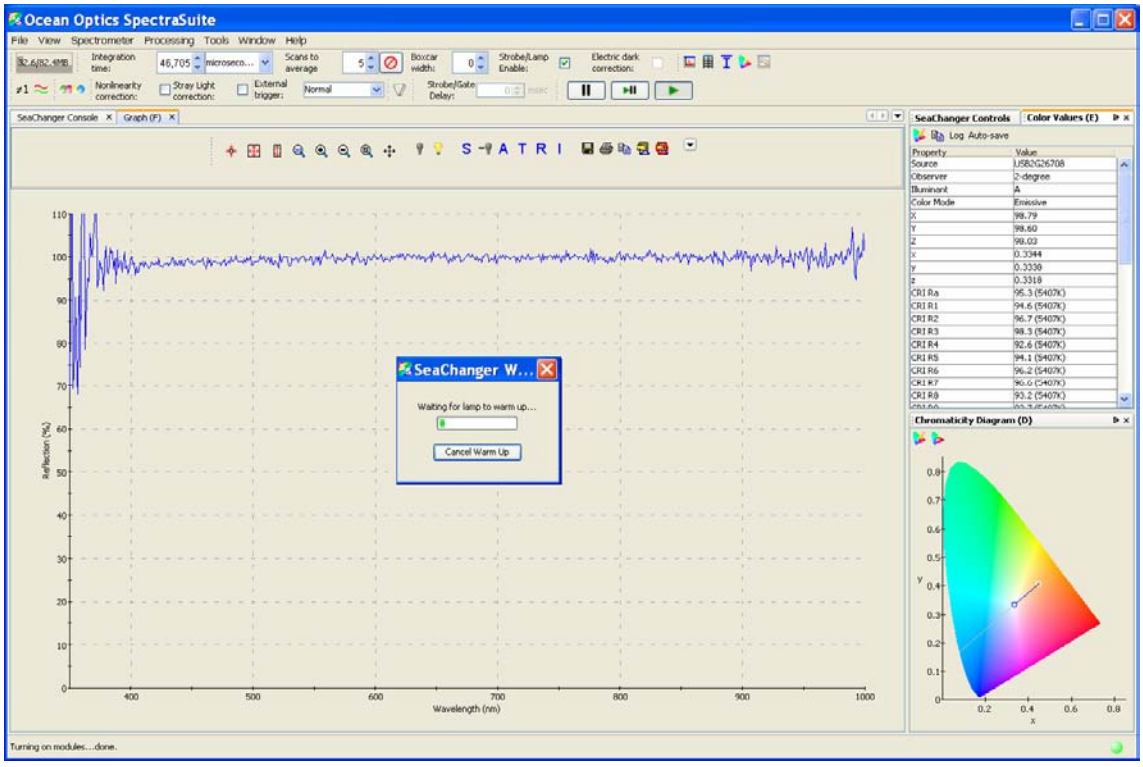
.

   a. If you selected None, go on to Step 3.

   b. If you selected LanBox DMX, the SeaChanger DMX Login dialog box appears. Enter the required information for the Ethernet connection to the LanBox-LCE.



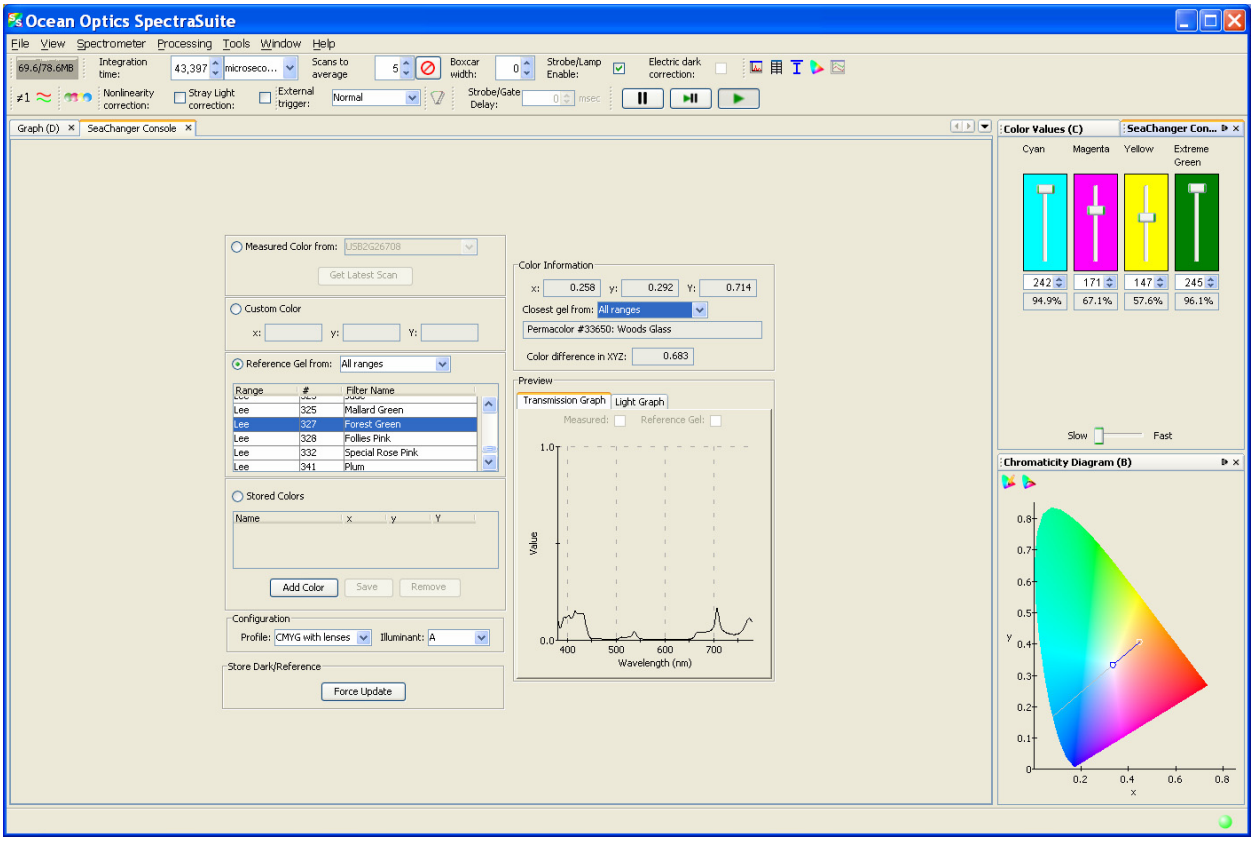
A graph appears with a message that the lamp is warming up.



During this time, an initialization process occurs in which SpectraSuite automatically does the following for you:

- Turns on the light source.
- Calibrates to the correct integration time.
- Stores a reference spectrum.
- Turns the lamp off to store a dark spectrum.
- Starts a transmission measurement.
- Adds a color measurement for emissive color.
- Starts the SeaChanger's LanBox DMX console and calibrates the measurements until they're stabilized.

3. The SeaChanger Console screen appears enabling you to change the parameters listed in the table below.



Parameter	Meaning
Measure Color from	Select the serial number of the spectrometer
Custom Color	Select a custom color
Reference Gel from	Select All ranges, Cinegel, Cinelux, Roscolux, Permacolor, or Lee

Parameter	Meaning
Stored Colors	Add, Save, Remove
Configuration	CYMG with lenses, CYMG w/o
Store Dark/Reference	Force Update
Color Information x , y, Y Closest gel from Color difference in XYZ	Select All ranges, Cinegel, Cinelux, Roscolux, Permacolor, or Lee
Preview	Allows you to preview the Transmission graph and the Light graph.

The controls in the upper right panel allow you to change the color of the SeaChanger by individually controlling its color wheels.

Testing

The Testing toolbar consists of the speed benchmark ( ). This feature allows you to see how fast the SpectraSuite application is running (how long it takes from the time the data is acquired until all the calculations have been performed. The Testing toolbar only displays when you select it with **View | Toolbars | Testing**; it is absent from the screen by default.

Trigger

The External Trigger selection box on the Trigger toolbar enables you to set the following trigger modes of the spectrometer:

Normal – free running

Software – Integration time is controlled by frequency of triggers

External Hardware – Hardware fixed or jumpered integration time

Strobe-Gate Delay

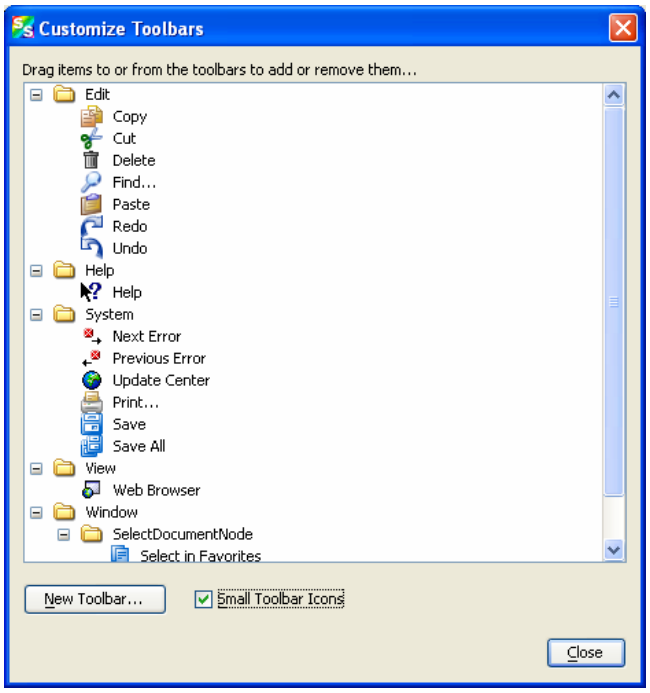
This control enables you to set the gating delay in msec.

Small Toolbar Icons

For future use.

Customize

This menu selection allows you to customize your toolbars with functions that you choose from the Customize Toolbars dialog box.



Chapter 6

Spectrometer Menu Functions

Overview

This chapter details the various options and functions available from the **Spectrometer** menu in SpectraSuite.

Acquisition

This menu selection consists of options that control starting and stopping SpectraSuite's acquisition of spectral data. If you have more than one acquisition running, you must select the desired spectrometer in the Data Sources pane. To do this, click on the line under the spectrometer that lists the integration time, scans to average and boxcar width.

Pause Acquisition/Resume Acquisition

These menu selections toggle to pause and restart data acquisition. When you start the SpectraSuite application, it comes up acquiring spectral data in Scope mode from the attached spectrometers. If you are monitoring more than one spectrometer, select the desired spectrometer in the Data Sources pane, and choose either **Spectrometer | Acquisition | Pause Acquisition** to temporarily pause the acquisition. Select **Spectrometer | Acquisition | Resume Acquisition** to resume the acquisition.

Terminate Acquisition

To completely stop spectral acquisition on a spectrometer, select the desired spectrometer in the Data Sources pane (if you are monitoring more than one), then select **Spectrometer | Acquisition | Terminate Acquisition.**

Spectrometer Features

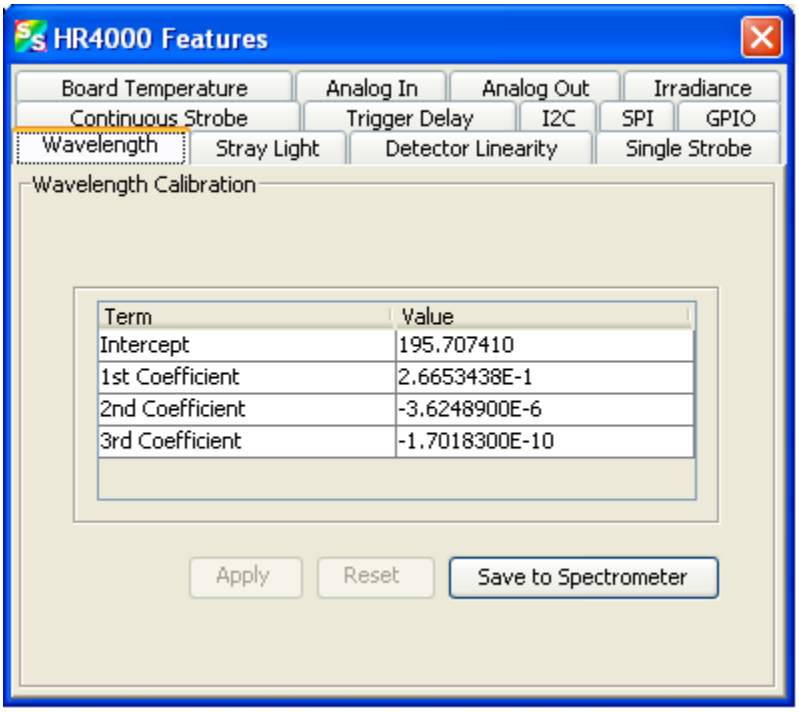
This option provides access to additional functionality available with the attached OOI spectrometers. You must select a spectrometer in the **Data Sources** pane to make this menu selection active. To display the Features dialog box, do one of the following:

Select **Spectrometer | Spectrometer Features** from the menu, or

Right-click on the device in the Data Sources pane and select **Spectrometer Features**.

Each attached device type has unique features, so see the documentation for your particular device to learn more about the available options and their settings. The MMS Raman Spectrometer has unique features. See *MMS Raman Spectrometer* for more information.

The following is an example of the HR4000 Spectrometer Features dialog box.



Many of the features listed for the HR4000 Spectrometer are also valid for other spectrometers. The table below lists all spectrometer features. Check your spectrometer to see which features apply to your model.

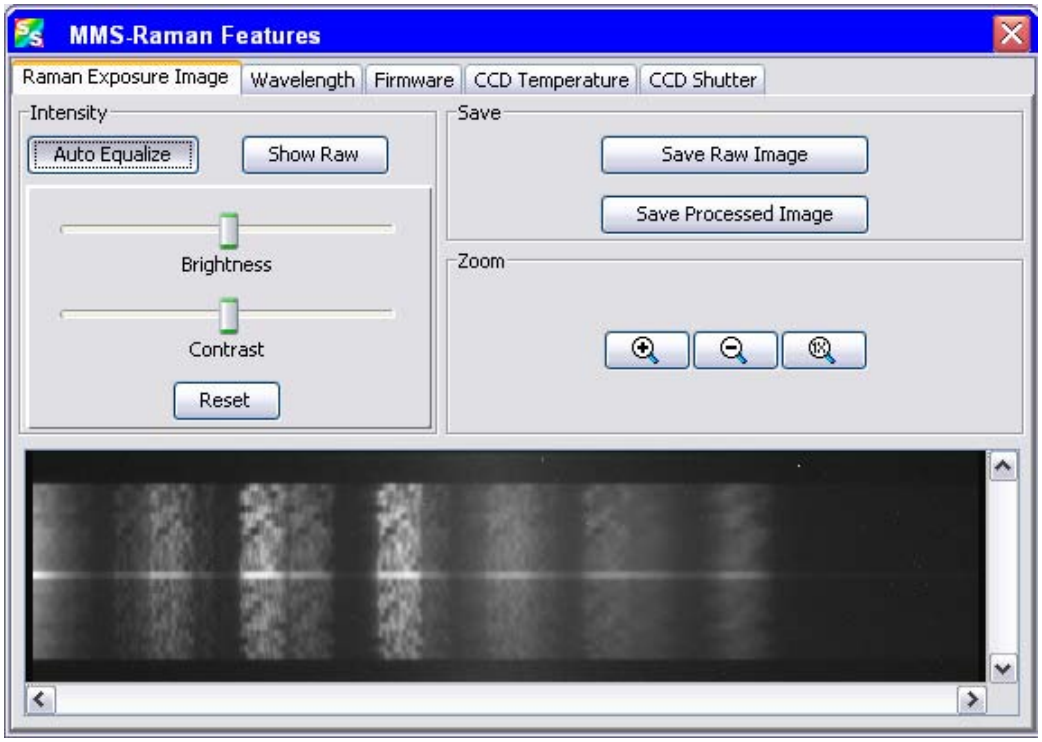
Feature	Meaning
Analog In	Set the input voltage and the update interval. Analog input can be accessed from the spectrometer's accessory connector.
Analog Out	Analog output can be used for multiple applications such as single pixel intensity analysis or programmable reference/dimmer to light sources. Set the analog output on this screen.

Feature	Meaning
Autonulling	Autonulling is an enhanced electrical dark correction. Set the autonulling status and value on this screen.
Board Temperature	The HR spectrometers contain a temperature sensor chip on the printed circuit board. Use this screen to set the temperature parameters.
Channel Features	For the ADC1000-USB. Enable each channel (1-7) by checking box.
Continuous Strobe	Set the continuous strobe delay. The Continuous Strobe signal is a programmable frequency pulse-train.
Detector Linearity	Use this screen to change the linearity coefficients.
External Trigger Delay	Set the counts for the external hardware trigger.
GPIO	Set the General Purpose Input/Output values on this screen.
Hardware Trigger	The spectrometer uses an external rising edge of a TTL signal to begin a single integration cycle. Set the delay (counts) on this screen.
I2C	The Inter-Integrated Circuit 2-wire serial bus is widely used in embedded systems applications. With I²C you can add peripherals to your system without using valuable resources like I/O ports. The I2C bus communications parameters are set on this screen.
Irradiance	Use this screen to load and save irradiance calibration factors.
LS-450	This tab appears if a USB-LS-450 light source is attached to your spectrometer. Check the box for Pulsed LED mode, if desired.
LS-450 Calibration Constants	This tab appears if a USB-LS-450 light source is attached to your spectrometer.
LS-450 Current Out	This tab appears if a USB-LS-450 light source is attached to your spectrometer. Adjust the analog output current.
Multi Channel Provider	This screen appears for an ADC1000.
Single Strobe	The Single Strobe signal is a programmable TTL pulse that occurs at a user determined time during each integration period. Set the counts for the high and low transition delay.
SPI	The Serial Peripheral Interface is a 3-wire interface that can be used to communicate to multiple slave devices. Access the SPI bus communications functions on this screen.
Stray Light	Enter the stray light correction coefficient in this screen.
TEC	For QE65000 spectrometers, set the parameters for the TE cooled

Feature	Meaning
	CCD array on this screen.
Thermoelectric	For NIR spectrometers.
Trigger Delay	Same as External Trigger Delay.
UV/VIS	ISS-UV-VIS Enable visible lamp, set visible lamp intensity, enable UV lamp, set UV lamp intensity
Wavelength	Allows you to enter or change the spectrometer's wavelength calibration coefficients. Wavelength coefficients are provided on the Wavelength Calibration Data Sheet that came with the spectrometer.

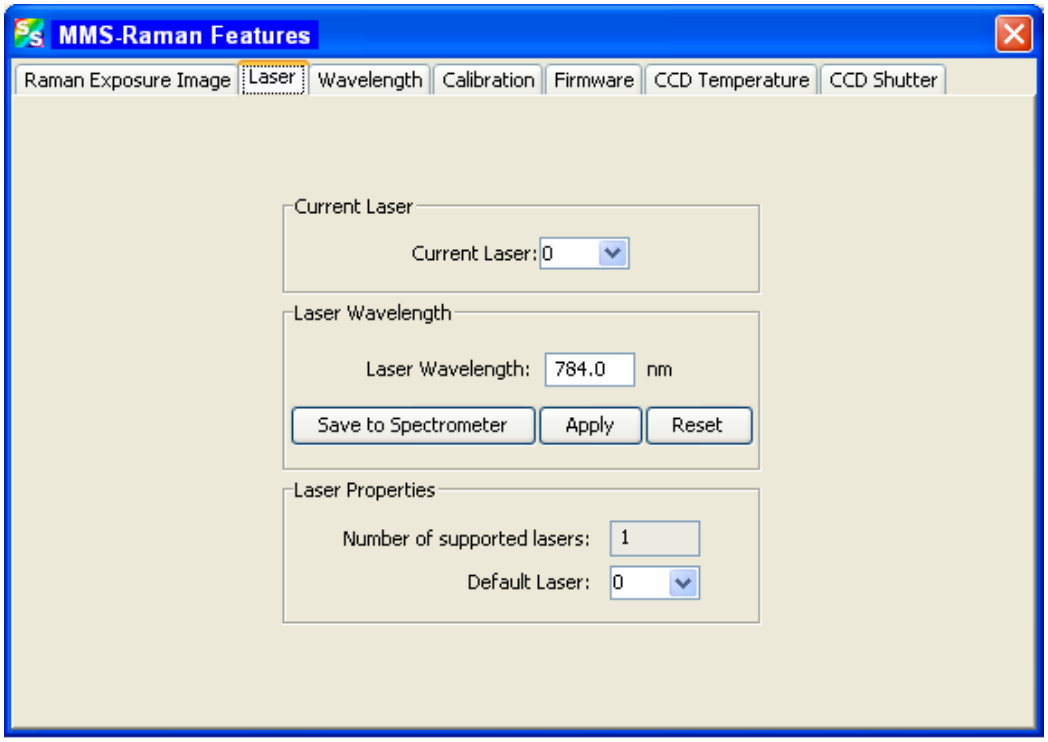
MMS Raman Spectrometer

The following are features for the MMS Raman Spectrometer:

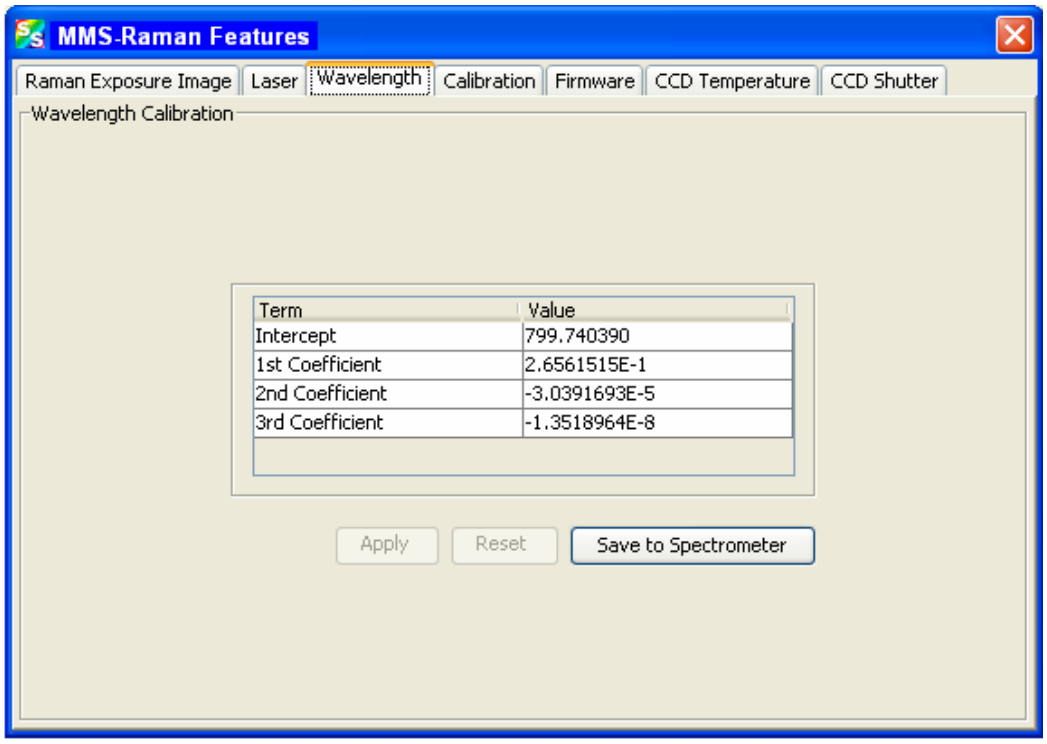


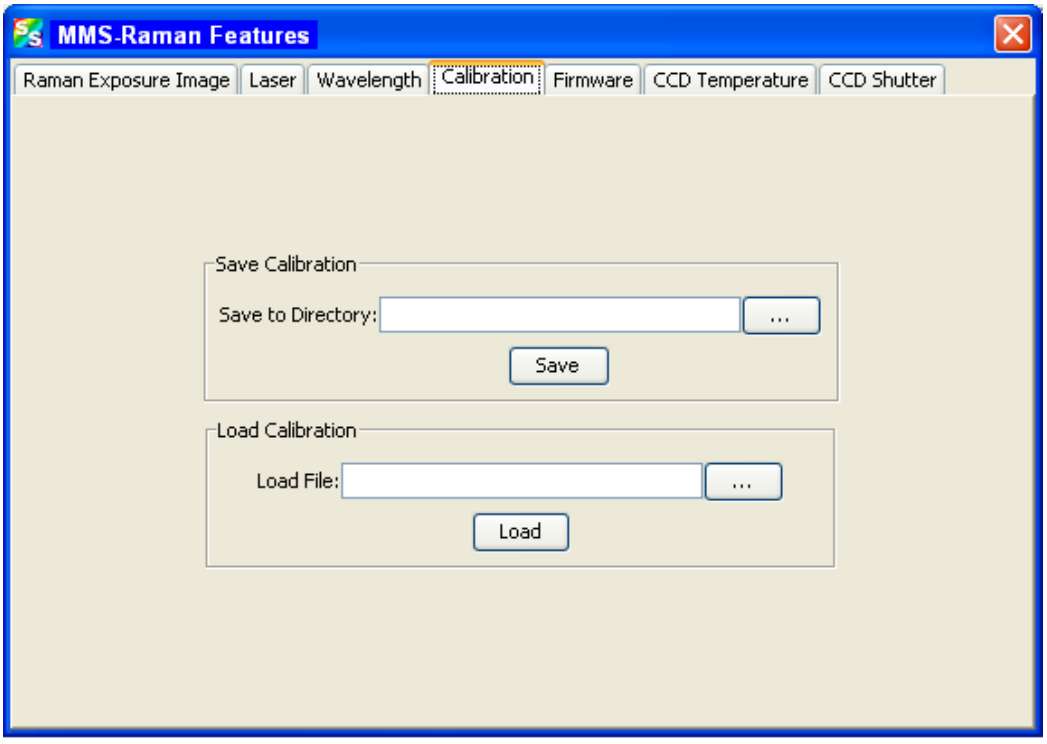
Use this screen to view the raw data coming from the chip (Raman exposure image) if your spectral graph looks incorrect. The bottom of this screen displays the actual CCD image (a 2-dimensional image of the detector). Each light stripe is a spectral line. The vertical white lines correspond to peaks.

Feature	Meaning
Auto Equalize	Use this adjust to get better contrast in the CCD image.
Show Raw	Displays the raw image.
Brightness/Contrast	Adjust the bright/contrast of the image.
Reset	Resets the image.
Save Raw Image/Processed Image	Save the raw/processed image to a file.
Zoom	Standard controls to zoom in/out

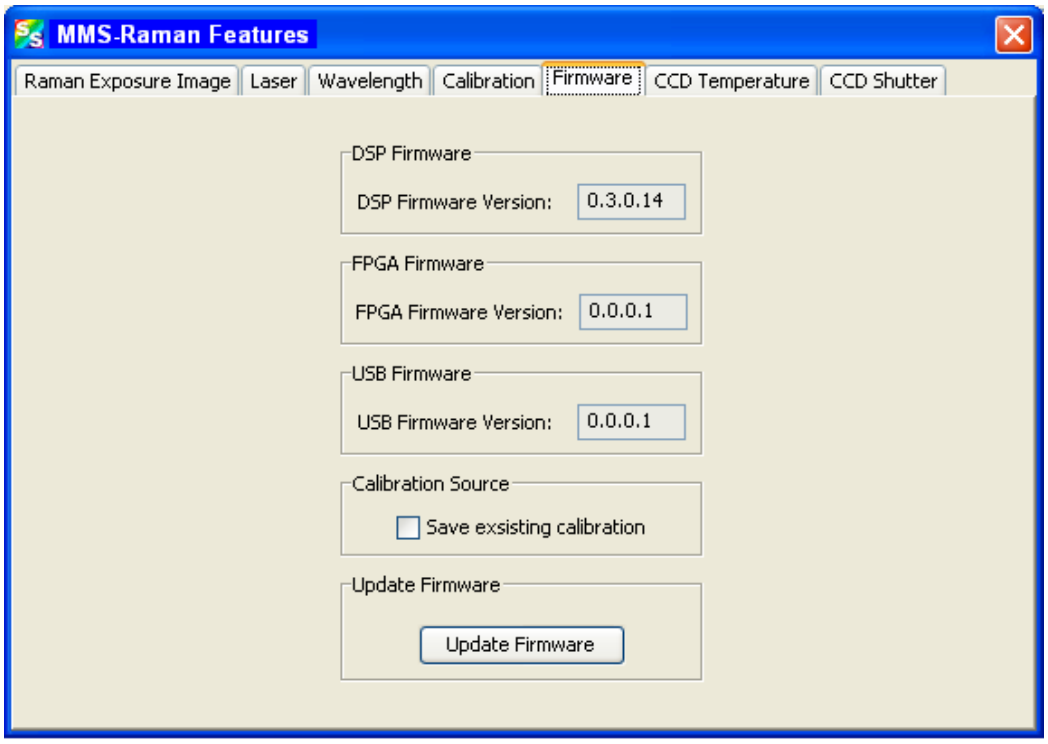


Use this screen to enter specific information for the laser being used.

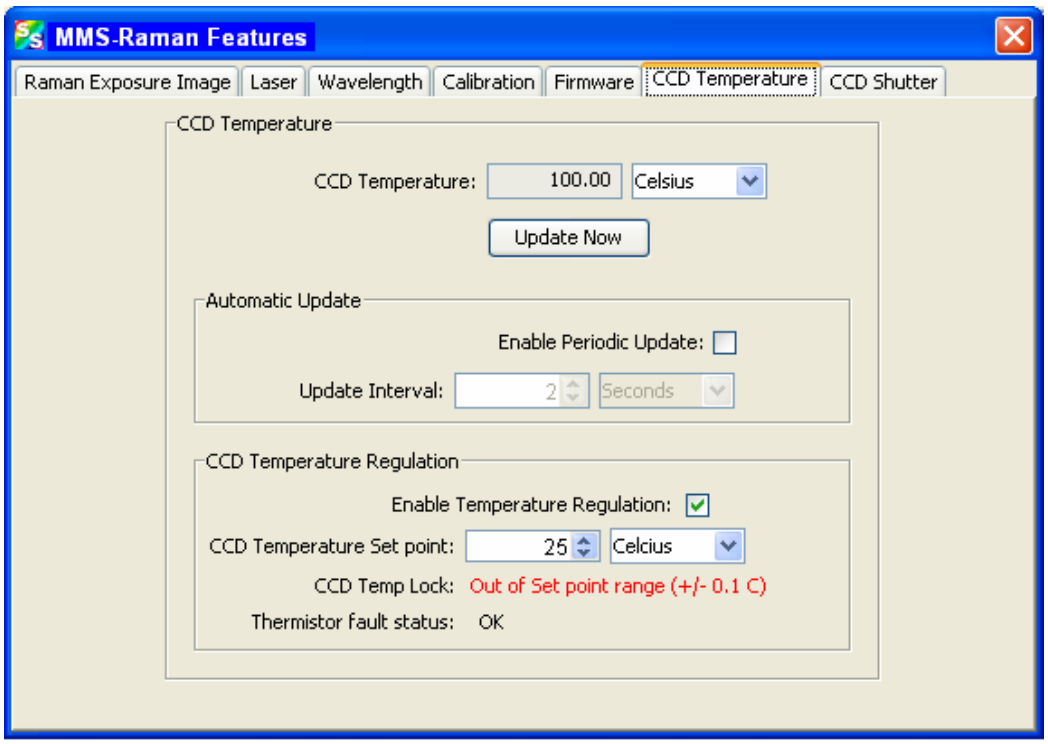




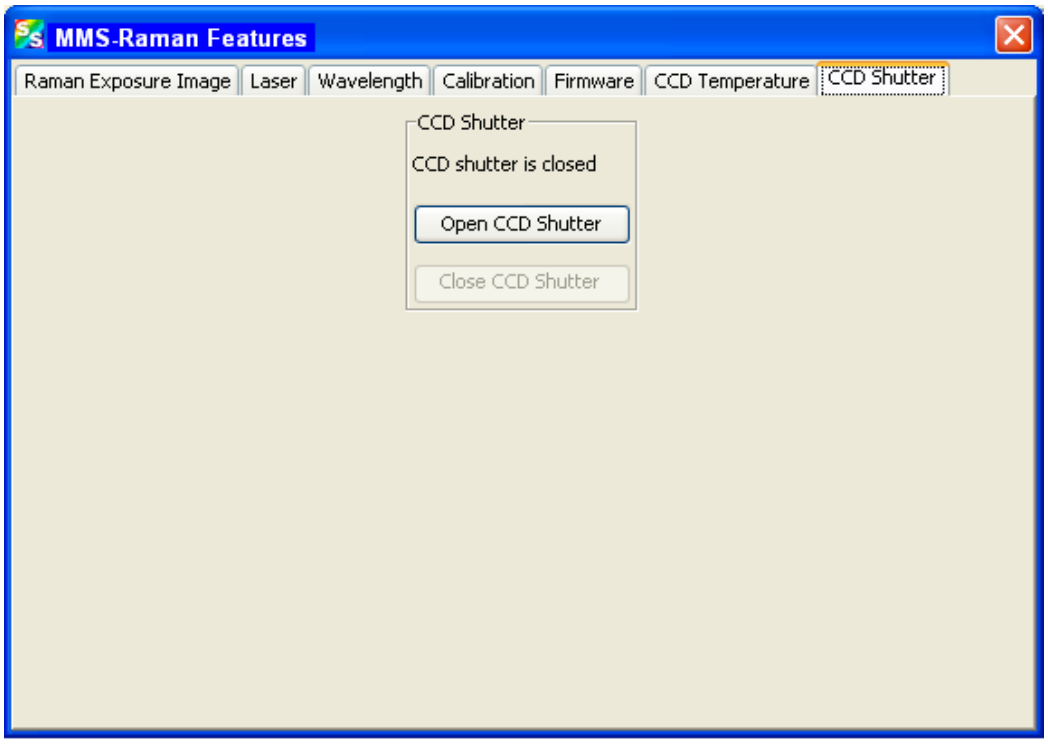
Use this screen to save or load calibration files.



Use this screen to update the firmware. You must stop all acquisitions before updating the firmware.



Use this screen to regulate the CCD temperature.



This feature allows you to control the CCD shutter. Close the shutter to store a dark spectrum.

Rescan Devices

Use this menu selection if you plug in a device after starting the SpectraSuite application. SpectraSuite then displays the new device in the Data Sources pane.

Remove Spectra

This menu selection deletes the captured high-speed spectra collection data. You can also right-click on the high-speed spectra collection icon in the **Data Views** pane and select **Remove Spectra**. See *High-Speed Acquisition* for more information.

Show Devices

This feature allows you to redisplay the Data Sources and Data Views panes if they have been closed.

Chapter 7

Processing Menu Functions

Overview

This section provides information on the various signal processing functions available under the Processing menu selection.

Color

Edit Color Settings

This menu item allows you to make changes to the color settings for color measurements.

Pre-processing

Preprocessing functions currently include the following:

Nonunity correction

Add Reference Monitor

You can also remove the preprocessing function.

Remove Preprocessor

Select **Processing | Pre-processing | Remove Preprocessor** to remove the nonunity correction preprocessing function.

Nonunity Correction

Select **Processing | Pre-processing | Non-unity correction** for reflection experiments if you need to perform a calculation to compensate for a reflection standard that is not perfectly white. You can also access this function with the icon in the Preprocessing toolbar.

Add Reference Monitor

Select **Processing | Pre-processing | Add Reference Monitor** to adjust the signal to compensate for variations in spectral intensity based on light source and system drift. The reference spectrum for the reference acquisition is the starting "ideal" state of the lamp. Any deviations the lamp makes from that reference spectrum will cause compensation in the sample acquisition.

For extended experiments, you will achieve optimal results if you take frequent reference spectra. If this is not possible, however, you can choose to monitor your light source and instruct SpectraSuite to correct for any drift that might occur. There are two types of drift: Spectrally uniform and spectrally nonuniform. The drift associated with a tungsten lamp is often spectrally uniform, but the drift associated with a deuterium lamp is not.

Reference Monitoring allows you to monitor a reference for variations in spectral intensity based on light source and system drift. To monitor a reference, the following conditions must be met:

You are using either multiple spectrometers (and spectra overlap in the area to be referenced), or one spectrometer with multiple acquisitions, and

You have stored both a reference and dark spectrum. Once these spectra have been stored, the Reference Monitoring function is activated (is available for use).

► *Procedure*

To perform reference monitoring:

1. Start an acquisition on the spectrometer that will monitor the lamp. Adjust the acquisition parameters so that the spectrum is on scale.
2. Store a reference and dark spectrum for that acquisition.
3. Start an acquisition on the spectrometer that will measure the sample.
4. Store a dark spectrum for the sample acquisition.
5. Click on the sample acquisition graph,

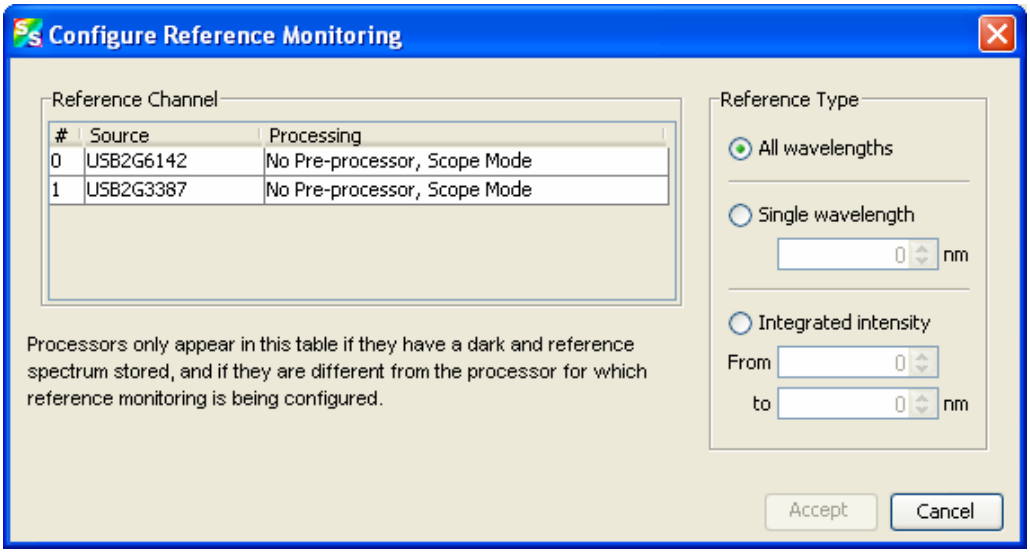
   Or,

   In the Data Sources pane, select the processing node for the sample acquisition (**No pre-processor**, etc.). The reference monitoring action should enable.

6. Click

   Or,

   Select **Processing | Preprocessing | Add Reference Monitor**. The **Configure Reference Monitoring** dialog box appears:


Configure Reference Monitoring
Reference Channel
Source Processing
0 USB2G6142 No Pre-processor, Scope Mode
1 USB2G3387 No Pre-processor, Scope Mode
Processors only appear in this table if they have a dark and reference spectrum stored, and if they are different from the processor for which reference monitoring is being configured.
Reference Type
All wavelengths
Single wavelength
0 nm
Integrated intensity
From 0
to 0 nm
Accept
Cancel

7. Select the desired reference channel.

8. Select the Reference Type as follows:

Selection	Meaning
All wavelengths	Requires a minimum of two spectrometer channels in your system, both configured for overlapping wavelength ranges. Corrects for both uniform and nonuniform drift.
Single wavelength	Use this selection for pixel-by pixel drift correction.
Integrated intensity	Use this selection if the lamp is going to drift uniformly

9. Click

.

Processing Mode

Processing mode functions include all of the modes necessary to conduct experiments. These modes are also available from the toolbar above the graph. See *Experiment Tutorials* for more information about how to conduct experiments using the processing modes.

Scope

Select **Processing | Processing Mode | Scope** to switch the current spectral window into Scope mode. You can also click in the graph's toolbar.

The signal graphed in Scope mode is the raw voltage coming out of the A/D converter. This spectral view mode provides complete control of signal processing functions before taking absorbance, transmission, reflection, and relative irradiance measurements. This mode reflects the intensity of the light source, the reflectivity of the grating and mirrors in the spectrometer, the transmission efficiency of the fibers, the response of the detector, and the spectral characteristics of the sample.

Use Scope mode when configuring your setup, adjusting the integration time, and taking a reference and a dark scan.

Scope Minus Dark

Select **Processing | Processing Mode | Scope Minus Dark** to switch the current spectral window into Scope mode and subtract the stored dark spectra from each spectrometer channel before SpectraSuite displays it. You can also click in the graph's toolbar.

See the description of Scope mode (*Scope*) for more information.

Absorbance

Select **Processing | Processing Mode | Absorbance** to switch the current window into Absorbance mode.

You can also click in the graph's toolbar. You must first store reference and dark spectra in Scope mode before you can access Absorbance mode.

SpectraSuite uses an equation to determine the concentration of a species in solution (illustrated below). The software uses this equation to evaluate each pixel on the detector and produce the absorbance spectrum:

$$A_\lambda = -\log_{10}\left(\frac{S_\lambda - D_\lambda}{R_\lambda - D_\lambda}\right)$$

Where:

S = Sample intensity at wavelength λ

D = Dark intensity at wavelength λ

R = Reference intensity at wavelength λ

The concentration of a species in a solution directly affects the absorbance of the solution. This relationship, known as Beer's Law, is expressed as:

$$A_\lambda = \varepsilon_\lambda c \ell$$

Where:

A = Absorbance at wavelength λ,

ε_λ = Extinction coefficient of the absorbing species at wavelength λ

c = Concentration of the absorbing species and ℓ is the optical path length of the absorption.

See *Experiment Tutorials* for information on conducting an experiment in Absorbance mode.

Transmission

Select **Processing | Processing Mode | Transmission** to switch the current window into Transmission mode. You can also click T in the graph's toolbar. This is also the spectral processing mode used for reflection spectroscopy, as the math necessary to compute reflection is identical to that required for transmission. You must first store reference and dark spectra in Scope mode before you can access Transmission mode.

SpectraSuite calculates the transmission of a solution using the following equation:

$$\%T_\lambda = \frac{S_\lambda - D_\lambda}{R_\lambda - D_\lambda} \times 100\%$$

Where:

S_λ = Sample intensity at wavelength λ

D_λ = Dark intensity at wavelength λ

R_λ = Reference intensity at wavelength λ

See *Experiment Tutorials* for information on conducting an experiment in Transmission mode.

Reflection

Select **Processing | Processing Mode | Reflection** to switch the current window into Reflection mode. You can also click R in the graph's toolbar. Reflection mode is also the spectral processing mode used for transmission spectroscopy, as the math necessary to compute transmission is identical to that required for reflection.

You must take reference and dark spectra in Scope mode before you can access Reflection mode.

SpectraSuite calculates the reflection of a solution using the following equation:

$$\%T_\lambda = \frac{S_\lambda - D_\lambda}{R_\lambda - D_\lambda} \times 100\%$$

Where:

S_λ = Sample intensity at wavelength λ

D_λ = Dark intensity at wavelength λ

R_λ = Reference intensity at wavelength λ

See *Experiment Tutorials* for information on conducting an experiment in Reflection mode.

Relative Irradiance

Select **Processing | Processing Mode | Relative Irradiance** to switch the current window into Relative Irradiance mode. You can also click I in the graph's toolbar.

Before you can access Relative Irradiance mode, you must take a reference spectrum in Scope mode of a blackbody of known color temperature. Additionally, you must obtain a dark spectrum by removing the fiber from the reference lamp and preventing light from entering it.

Relative irradiance spectra are a measure of the intensity of a light source relative to a reference emission source. SpectraSuite calculates relative irradiance using the following equation:

$$I_\lambda = B_\lambda \left(\frac{S_\lambda - D_\lambda}{R_\lambda - D_\lambda} \right)$$

Where:

B_λ = Relative energy of the reference calculated from the color temperature

S_λ = Sample intensity at wavelength λ

D_λ = Dark intensity at wavelength λ

R_λ = Reference intensity at wavelength λ

See *Experiment Tutorials* for information on conducting an experiment in Relative Irradiance mode.

Raman Shifts

Use this menu item when you are doing Raman spectroscopy. This is the distance from the excitation source. You must have entered the wavelength of your laser (see *Set Laser Wavelength*) to use Raman Shifts.

Absolute Irradiance

Irradiance is the amount of light present on a particular area, such as the fiber's cross-section at its tip, a cosine corrector's surface, or the integrating sphere's surface (measures the total optical output of a light source inserted into the integrating sphere).

Scope

This menu selection allows you to completely control signal processing prior to calibrating the spectral response of your system and taking measurements. Use caution when operating in Scope mode since this mode represents a combination of several factors such as the intensity of the light source, the reflectivity of the grating and mirrors in the spectrometer, the transmission quality of the fibers, the response of the detector, and the spectral characteristics of the sample.

Absolute Irradiance

Select **Processing | Absolute Irradiance | Absolute Irradiance** to create a new graph of spectral data Absolute Irradiance mode. You can also click in the Data Display toolbar to use the wizard to create an Absolute Irradiance graph.

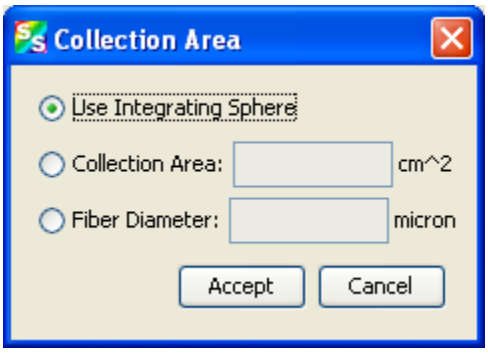
Absolute Irradiance Mode calculates the true irradiance of a spectrum, displayed in actual µW/cm^2/nm (or µW/nm when using an integrating sphere) incident on the probe's collection area. You do not need to store reference spectrum first since absolute irradiance is not relative to another measurement. However, you must store a dark spectrum and have a calibration file before you can measure absolute irradiance.

If your spectrometer was calibrated by Ocean Optics, you should have received a CD containing the Radiometric Calibration Files specific to your spectrometer. If you do not have these files, then you must create your own spectrometer calibration files using calibrated light sources that have lamp files for absolute irradiance.

See *Experiment Tutorials* for information on conducting an experiment in Absolute Irradiance mode.

Collection Area

Select **Processing | Absolute Irradiance | Collection Area** to enter the specifications of the collection area.



The Collection Area dialog box offers the following options:

Use Integrating Sphere – Enable this option only if you have an integrating sphere and use the LS1-CAL-INT calibrated light source. (In this case the source is inside the sphere and there is no collection area associated normally with a probe.) When this box is enabled and you are using the integrating sphere to collect light externally (source is outside the integrating sphere), SpectraSuite assumes the value in the **Fiber Diameter** field is the diameter of the opening in the integrating sphere. Be sure to enter the correct value (in microns).

Collection Area – If you know the actual collection area, enter it here. The default is 1.

Fiber Diameter – If the tip of a fiber is used as the collection probe, enter the bare fiber's diameter in microns. If an integrating sphere is used to collect light from a surface, enter the sphere's opening diameter (in microns). However, if a light source is inserted into the sphere, this value is ignored. If a cosine corrector is used, define the light collection area as follows:

If this cosine corrector is used . . .	Enter this diameter (in um) . . .
CC-3 or CC-3-UV	3900
CC-3-DA	7140

SpectraSuite then calculates the collection area from the fiber diameter.

Calibration

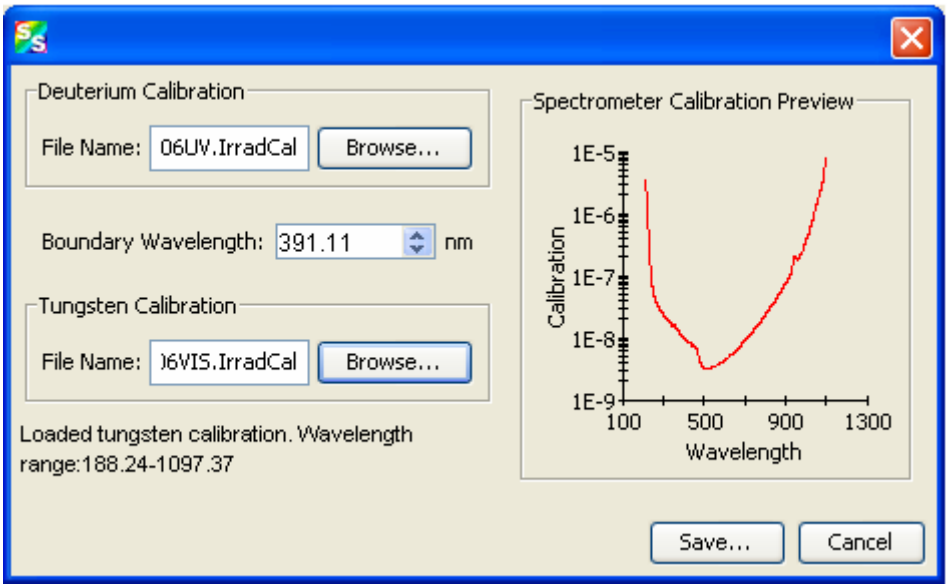
You can calibrate your spectrometer in two ways:

Ocean Optics can calibrate the spectrometer for you and send you the resulting calibration file, or

You can calibrate the spectrometer yourself using a light source (calibration lamp) with known spectral output (microwatts per square centimeter per nanometer) using this menu item.

Combine Calibration Files

This feature allows you to combine two spectrometer calibration files ***that you have created***; one file using a calibrated deuterium lamp source (UV) and the other using a calibrated tungsten lamp source (VIS). This will result in a spectrometer calibration file that can be used across the entire spectral range.



► *Procedure*

1. Select **Processing | Absolute Irradiance | Combine Calibration Files**.
2. Enter the file name of the spectrometer calibration file you created with the deuterium lamp source or browse to the desired file.
3. Enter the file name of the spectrometer calibration file that you created with a tungsten lamp source or browse to the desired file.
4. In the Boundary Wavelength field, select the wavelength at which point the two files will be joined or go on to Step 5 to just accept the value provided by SpectraSuite.
5. Click Save... . The graph of the combined files appears in the **Spectrometer Calibration Preview**.

New Energy, Power, Photons

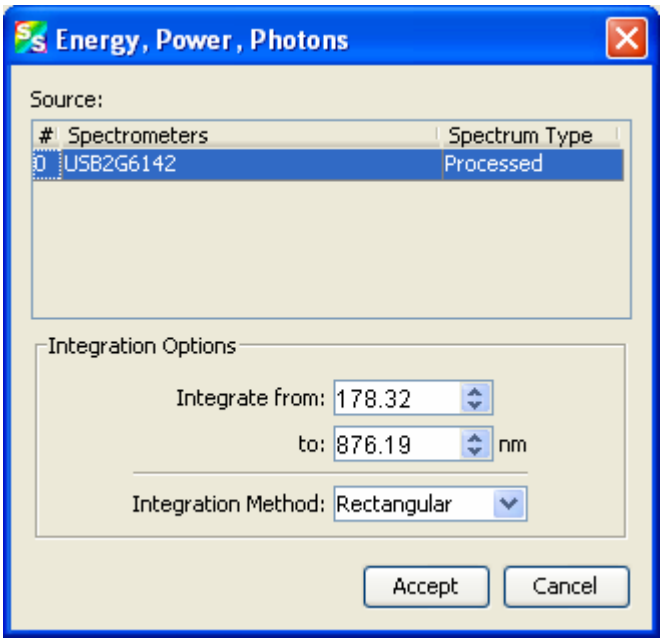
This feature enables you to measure integrated intensities. Radiometric values require that you specify the wavelength range. You must be in Absolute Irradiance mode (click) for this menu selection to be active.

► *Procedure*

1. Create a new graph of spectral data in Absolute Irradiance mode. See *Absolute Irradiance* in Appendix A: *Experiment Tutorials* for detailed instructions.
2. Select **Processing | Absolute Irradiance | New Energy, Power, Photons** to display the Energy, Power, Photons dialog box.

   OR

   Click on an Absolute Irradiance graph.



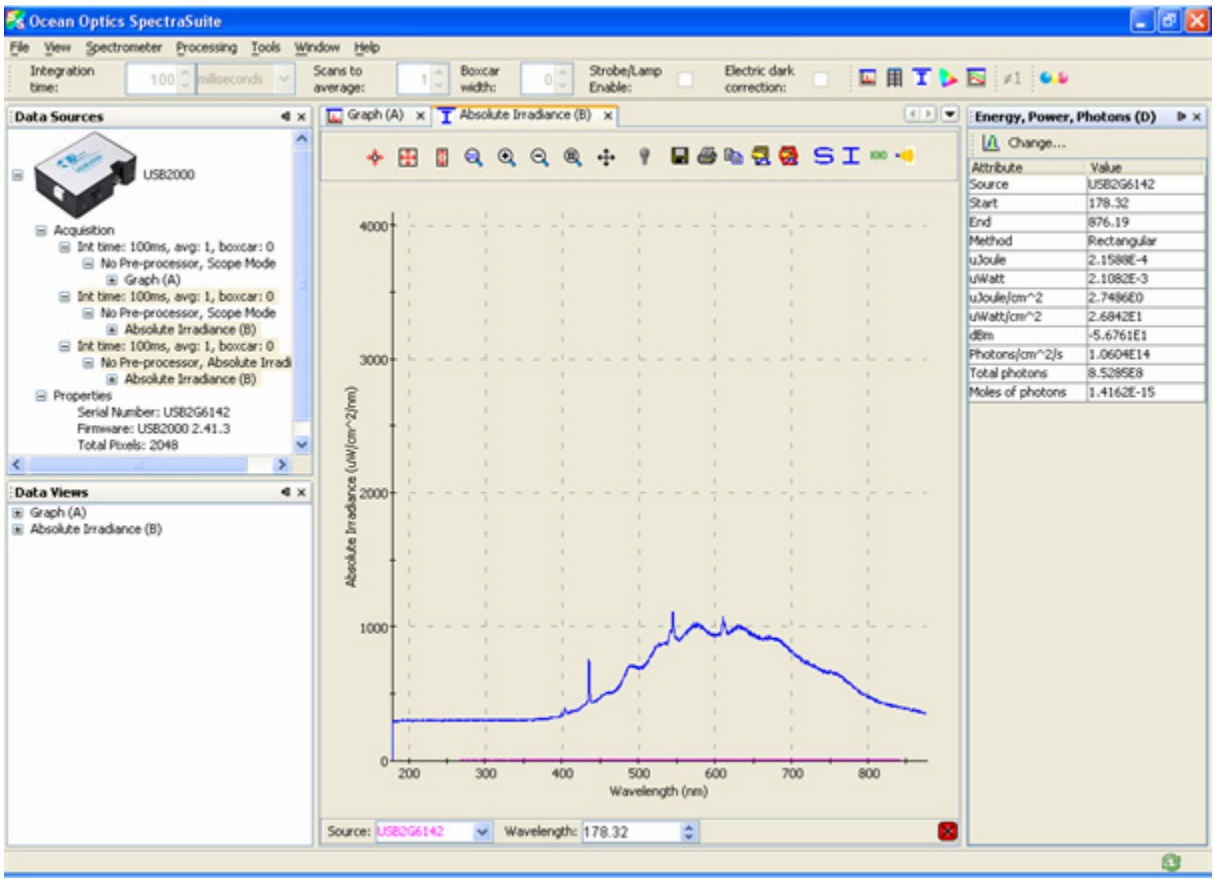
3. If more than one Absolute Irradiance graph is open, select the desired spectrometer by highlighting it under **Source**.

4. Enter the wavelength range to integrate in the Integration Options section.

5. Enter the **Integration Method**, either Rectangular, Simpson's (Rule), or Trapezoid.

6. Click

when finished. The Energy, Power, Photons table appears to the right of the graph. You can change these values by clicking the Change icon ( ) in the Energy, Power, Photons table.



This table is described below:

Attribute	Meaning
Source	The absolute irradiance source you selected in Step 3.
Start	The starting wavelength you selected in Step 4.
End	The ending wavelength you selected in Step 4.
Method	The integration method you selected in Step 5.
µJoule	The calculated energy of the sample in microjoules.
µWatt	The calculated power of the sample in microwatts.
µJoule/cm^2	The calculated energy per square centimeter of the sample.
µWatt/cm^2	The calculated power per square centimeter of the sample.
dBm	The decibels referenced to one milliwatt. Used to calculate power for lasers.
Photons/cm^2/s	The number of photons per square centimeter emitted from the sample each second.

Attribute	Meaning
Total photons	The total number of photons calculated.
Moles of photons	The moles of photons calculated.

New Photometry Measurement

This menu selection enables you to take photometry measurements such as lumen, lux, and candela. Phototropic/Scotopic values are calculated over a 380 to 780 nm wavelength range. Scotopic conditions are defined when the luminance is less than some hundredths of a candela per square meter (cd/m^2). The difference between this scotopic vision (low-level condition) compared to a photopic (high-level condition) affects the calculations for Lumen, Lux, and Candela by using the V'(λ) spectral luminous efficiency curve instead of the V(λ) curve.

You must be in Absolute Irradiance mode (click) for this menu selection to be active.

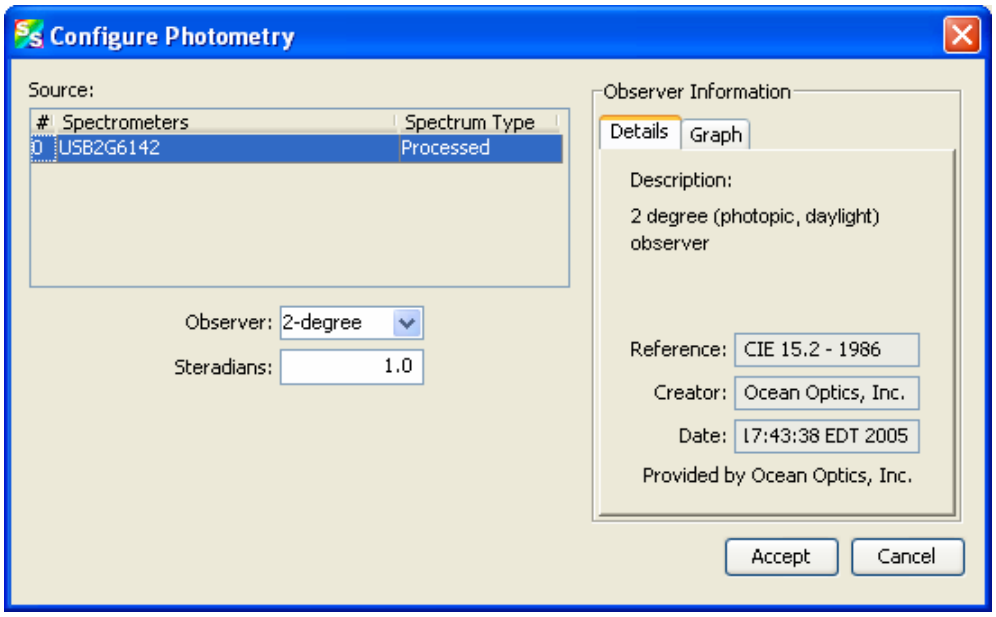
► *Procedure*

1. Create a new graph of spectral data in Absolute Irradiance mode. See *Absolute Irradiance* in Appendix A: *Experiment Tutorials* for detailed instructions.

2. Select **Processing | Absolute Irradiance | New Photometry Measurement** to display the **Configure Photometry** dialog box.

   OR

   Click on an Absolute Irradiance graph.

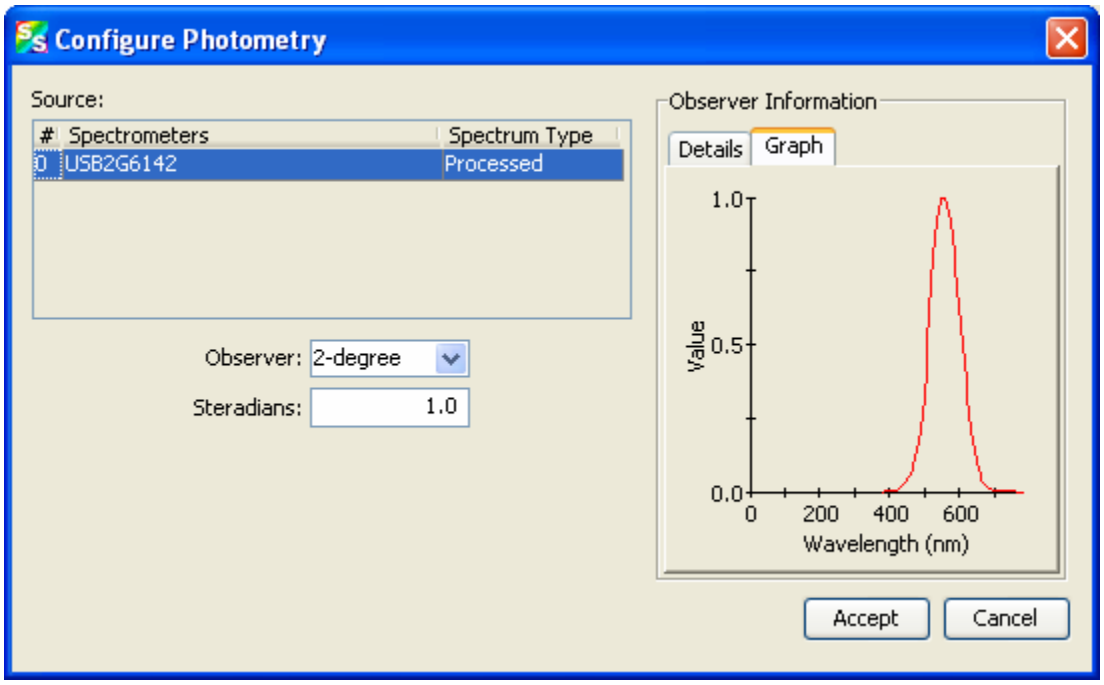


3. If more than one Absolute Irradiance graph is open, select the desired spectrometer by highlighting it under **Source**.

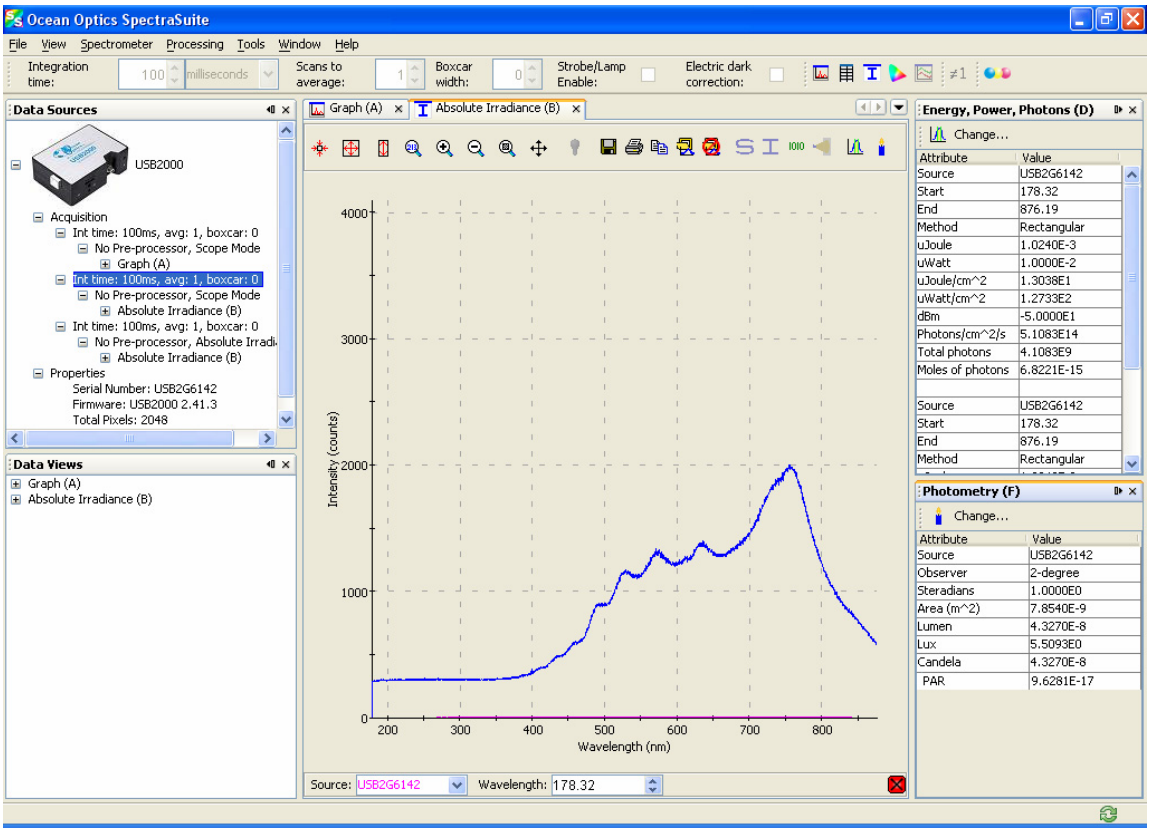
4. Select the **Observer** from the drop-down list.

5. Use the default **Steradians** (1.0) or enter your own value. (If the steradians value is 1, then candela = lumens).

   The right section of the dialog box displays Observer Information in Detail or Graph form (Graph form is shown below, Detail form is shown on the previous page).



6. Click . The Photometry table appears to the right of the graph. You can change these values by clicking the Change icon ( ) in the Photometry table.



The Photometry table is described below:

Attribute	Meaning
Source	The absolute irradiance source you selected in Step 3.
Observer	The type of observer you chose in Step 5.
Steradians	A unit of measurement used to describe the solid angle of a cone from the surface of a sphere to the center of the sphere. It is a solid angular measurement used when calculating illumination. The Lumens value is divided by the Steradians value to obtain Candela.
Area (m^2)	The light collection area per meter squared.
Lumen	The lumen value. A lumen is a “light watt.” Lumens are calculated as the absolute spectral response of the human eye.
Lux	The lux values. The lux value is obtained by calculating the lumen per square meter. Lux is also called a meter candle.
Candela	The luminous intensity of the sample, based on international standards.
PAR	Photosynthetic Active Radiation. The number of moles of photons between 400 -- 700 nm measured by absolute irradiance. To vary the 400-700 nm range, you can specify the moles of photons range using *New Energy, Power, Photons*.

X-axis Units

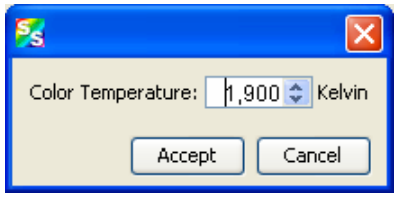
This menu item allows you to select the units for the x-axis on the spectrum graph. Choose from Gigahertz, Microns, Pixels, Raman Shifts, Nanometers, and Wavenumbers. The default value is Wavelength (nm).

Set Color Temperature

Setting the color temperature is useful if you have a lamp and you know what its temperature is. You can use the lamp color temperature that you set here when doing a color measurement (see *Fluorescence*).

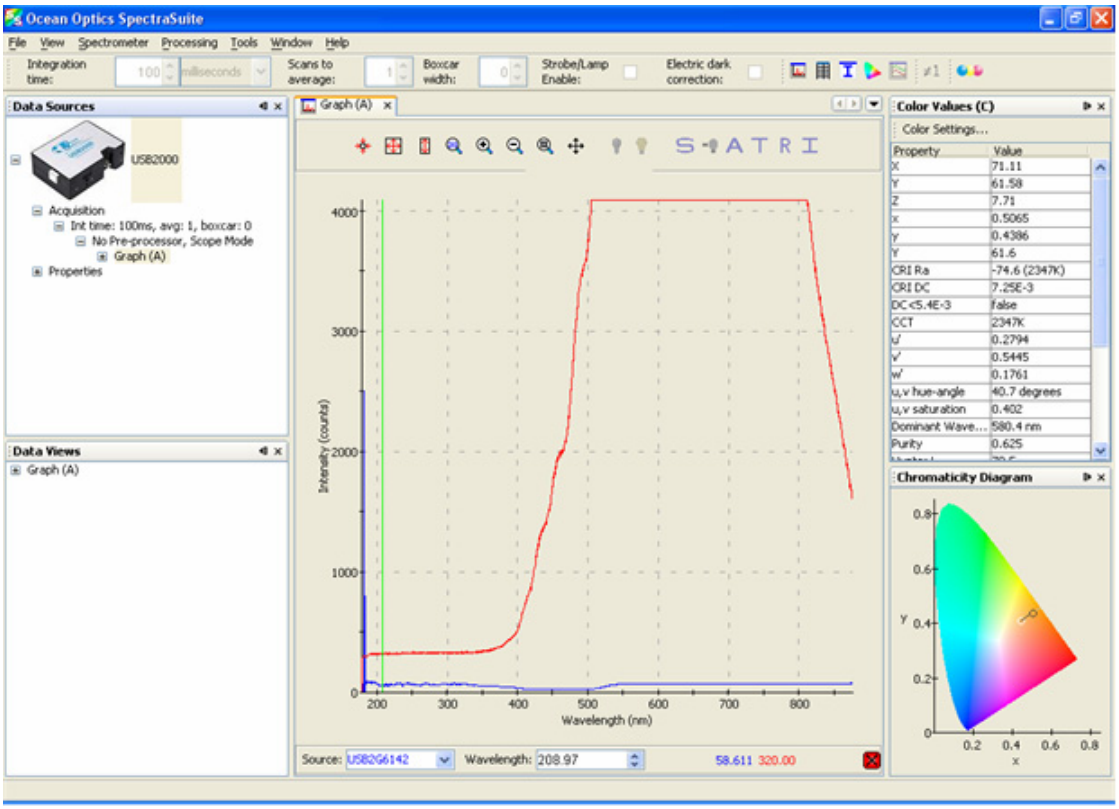
► *Procedure*

1. Select **Processing | Select Color Temperature** to display the Configure Photometry dialog box.



2. Set the desired color temperature (in Kelvin) and click

. The color value that you set here appears in the Color Values pane of the Color Measurement window.

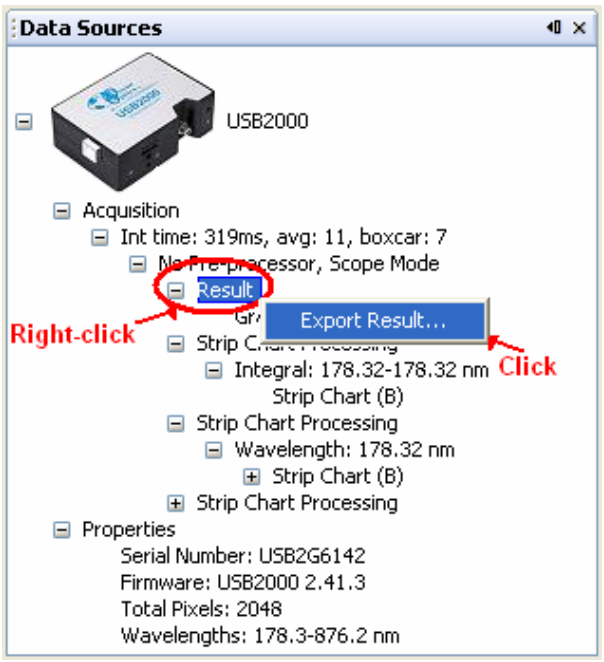


Exporting Processed Data

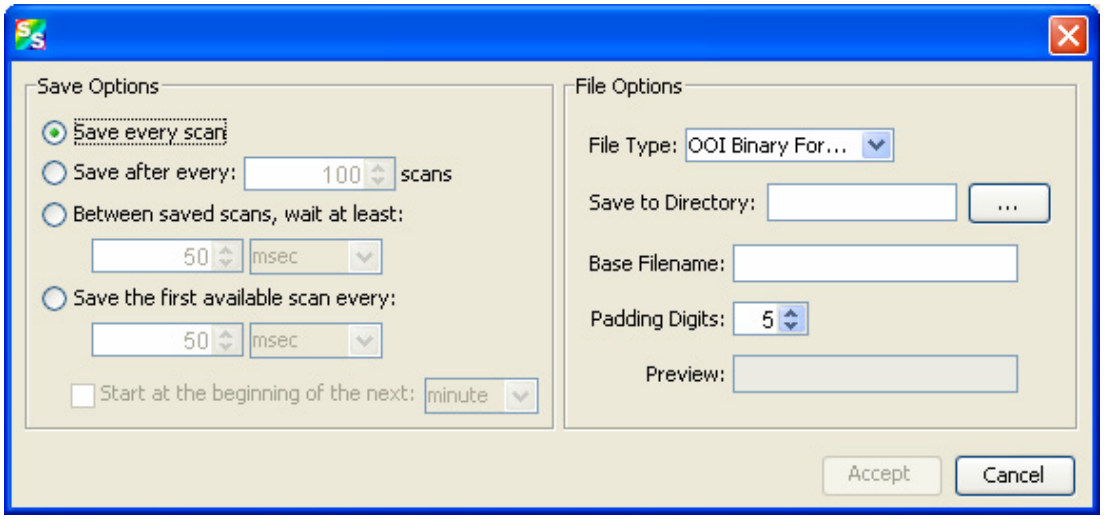
SpectraSuite provides the capability of saving and exporting processed data to a binary or tab-delimited file. When combined with external triggering, this feature can be used to automatically save full spectra timed to one or more external events.

► *Procedure*

1. Right-click on **Result** in the tree in the Data Sources pane and select **Export Result**.



The dialog box for exporting data appears.

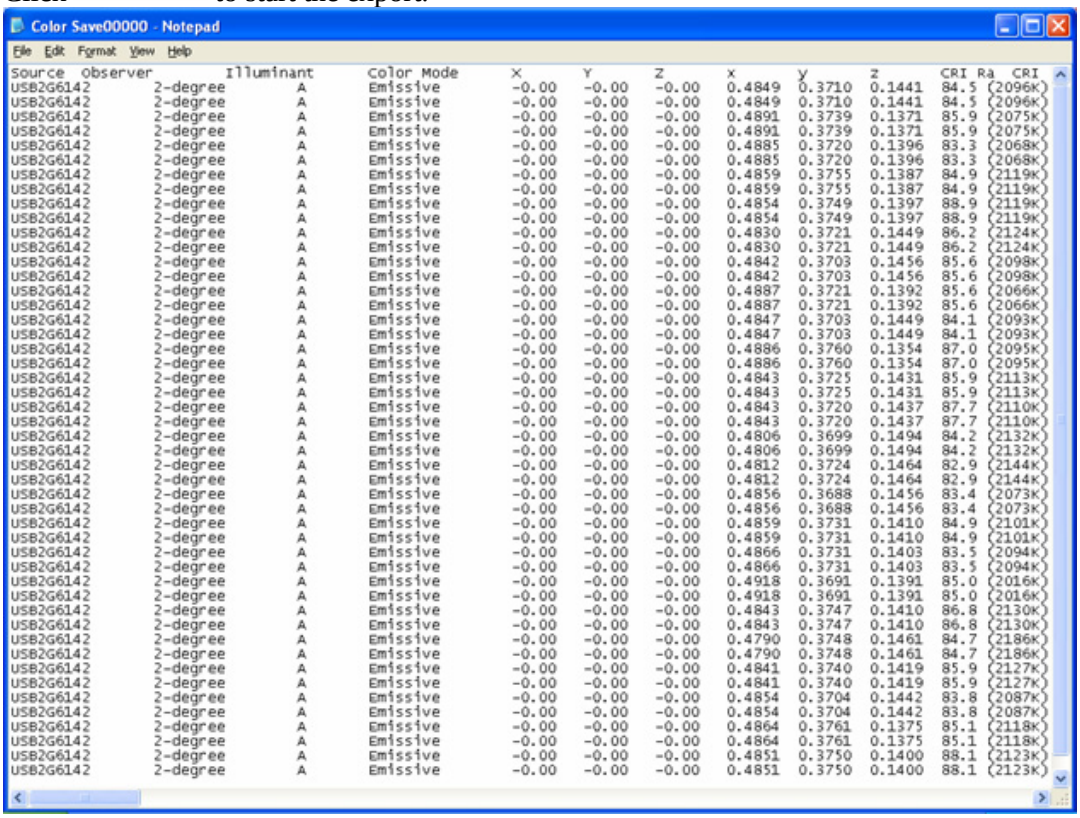


2. Enter the following information:

Field	Selections
Save options: Save every scan Save after every: x scans	Saves: Every scan After every *x* scans

Field	Selections
Between saved scans, wait at least:	Scans that occur at the interval selected
Save the first available scan every	The first scan that occurs after the interval selected
File options:	Enter:
File Type	Grams SPC, JCAMP, OOI Binary Format or Tab Delimited
Save to directory	The desired directory or browse to the desired directory
Base Filename	The name of the files
Padding Digits	Enter the number of digits to be used when appending to a file (enter 3 to save hundreds of files, enter 4 to save thousands, etc. up to 15), for example: spectrumfile001 through spectrumfile999 if 3 is selected
Preview	For future use

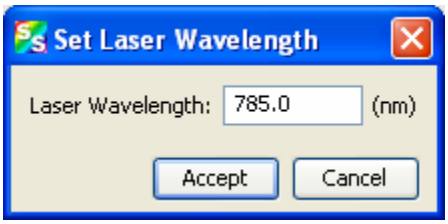
3. Click Accept to start the export.



Source	Observer	Illuminant	Color Mode	X	Y	Z	x	y	z	CRI Ra	CRI
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4849	0.3710	0.1441	84.5	(2096K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4849	0.3710	0.1441	84.5	(2096K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4891	0.3739	0.1371	85.9	(2075K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4891	0.3739	0.1371	85.9	(2075K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4885	0.3720	0.1396	83.3	(2068K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4885	0.3720	0.1396	83.3	(2068K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4859	0.3755	0.1387	84.9	(2119K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4859	0.3755	0.1387	84.9	(2119K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4854	0.3749	0.1397	88.9	(2119K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4854	0.3749	0.1397	88.9	(2119K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4830	0.3721	0.1449	86.2	(2124K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4830	0.3721	0.1449	86.2	(2124K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4842	0.3703	0.1456	85.6	(2098K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4842	0.3703	0.1456	85.6	(2098K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4887	0.3721	0.1392	85.6	(2066K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4887	0.3721	0.1392	85.6	(2066K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4847	0.3703	0.1449	84.1	(2093K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4847	0.3703	0.1449	84.1	(2093K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4886	0.3760	0.1354	87.0	(2095K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4886	0.3760	0.1354	87.0	(2095K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4843	0.3725	0.1431	85.9	(2113K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4843	0.3725	0.1431	85.9	(2113K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4843	0.3720	0.1437	87.7	(2110K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4843	0.3720	0.1437	87.7	(2110K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4806	0.3699	0.1494	84.2	(2132K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4806	0.3699	0.1494	84.2	(2132K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4812	0.3724	0.1464	82.9	(2144K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4812	0.3724	0.1464	82.9	(2144K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4856	0.3688	0.1456	83.4	(2073K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4856	0.3688	0.1456	83.4	(2073K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4859	0.3731	0.1410	84.9	(2101K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4859	0.3731	0.1410	84.9	(2101K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4866	0.3731	0.1403	83.5	(2094K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4866	0.3731	0.1403	83.5	(2094K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4918	0.3691	0.1391	85.0	(2016K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4918	0.3691	0.1391	85.0	(2016K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4843	0.3747	0.1410	86.8	(2130K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4843	0.3747	0.1410	86.8	(2130K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4790	0.3748	0.1461	84.7	(2186K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4790	0.3748	0.1461	84.7	(2186K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4841	0.3740	0.1419	85.9	(2127K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4841	0.3740	0.1419	85.9	(2127K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4854	0.3704	0.1442	83.8	(2087K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4854	0.3704	0.1442	83.8	(2087K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4864	0.3761	0.1375	85.1	(2118K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4864	0.3761	0.1375	85.1	(2118K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4851	0.3750	0.1400	88.1	(2123K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4851	0.3750	0.1400	88.1	(2123K)

Set Laser Wavelength

Use this menu item when you are doing Raman spectroscopy. Enter the wavelength of the laser you are using. You must enter a wavelength before you can access the Raman Shifts menu item. See *Raman Shifts* for more information.

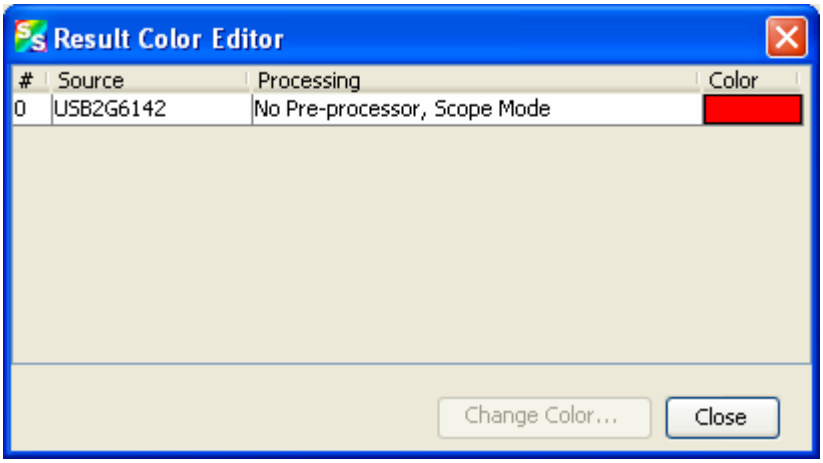


Edit Result Colors

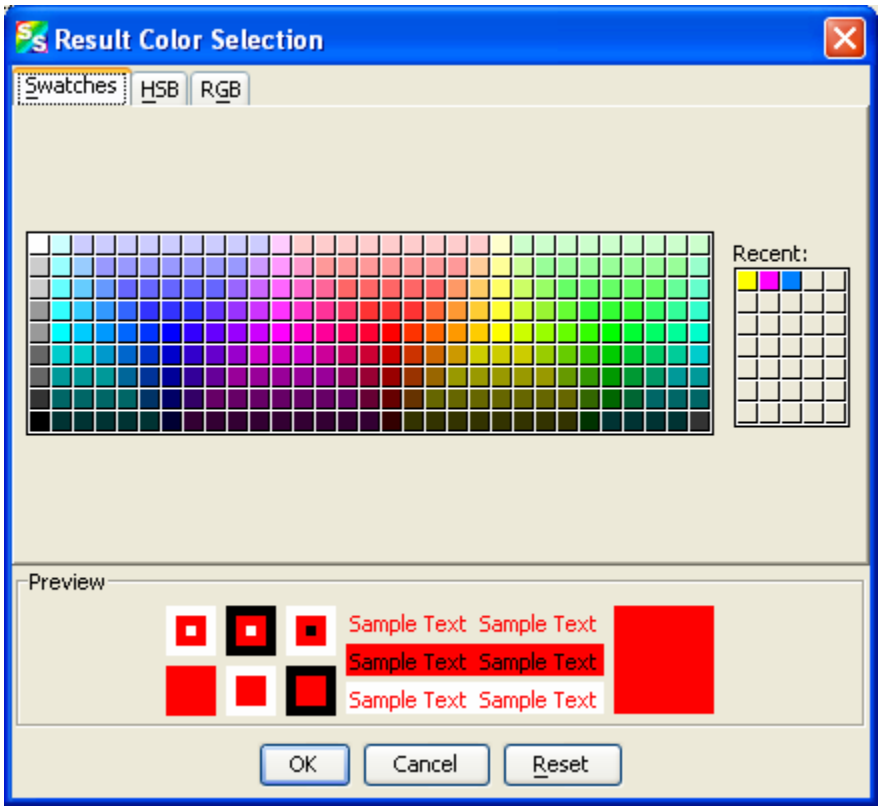
This function allows you to choose the color in which your data is displayed. The color selected will apply to all graphs in which that data appears, including Absolute Irradiance and Strip Charts.

► *Procedure*

1. Select **Processing | Edit Result Colors** to display the Result Color Editor dialog box.



2. Highlight the desired source and click **Change Color**. The Result Color Selection dialog box appears.



This dialog box provides three methods of selecting color -- by swatches, HSB (hue, saturation and brightness), or RGB (red, green, blue)..

3. Select the tab corresponding to the color selection method you wish to use.

4. Select the desired color. The **Recent** graphic lists any colors that you have recently chosen. You can select one of the recent colors instead of creating a new one. Once you have selected a color, the Preview panel displays an example of the color you have chosen.

   If the color is what you want, click the **OK** button. If you wish to reselect the original color, click the **Reset** button, then click **OK**.

5. The screen returns to the Result Color Editor dialog box. Click **Close**. The graph now displays in the selected color.

Chapter 8

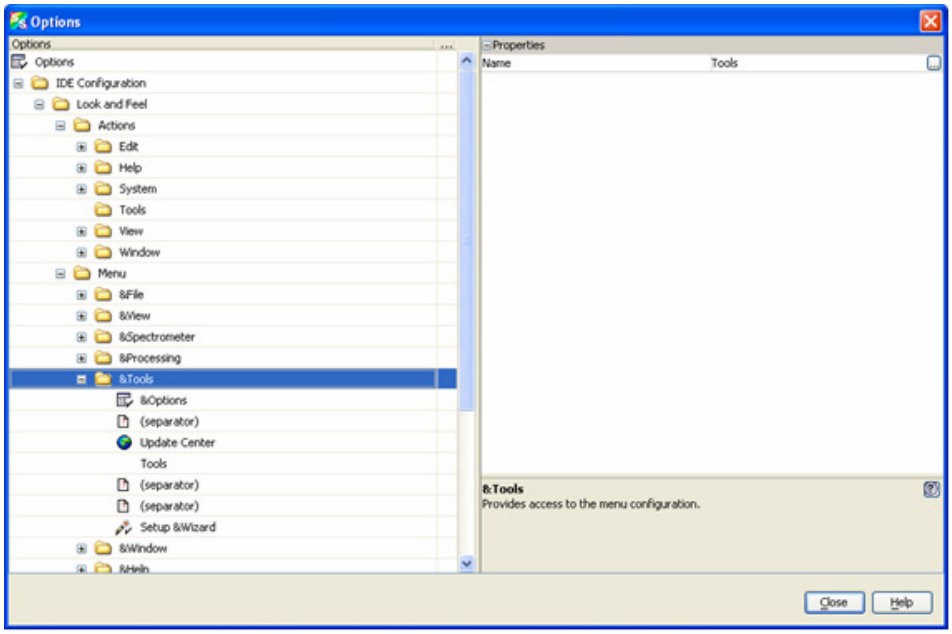
Tools Menu Functions

Overview

The tools menu provides the functionality to access the update center, select NetBeans settings for SpectraSuite modules, and to control the SpectraSuite parameters.

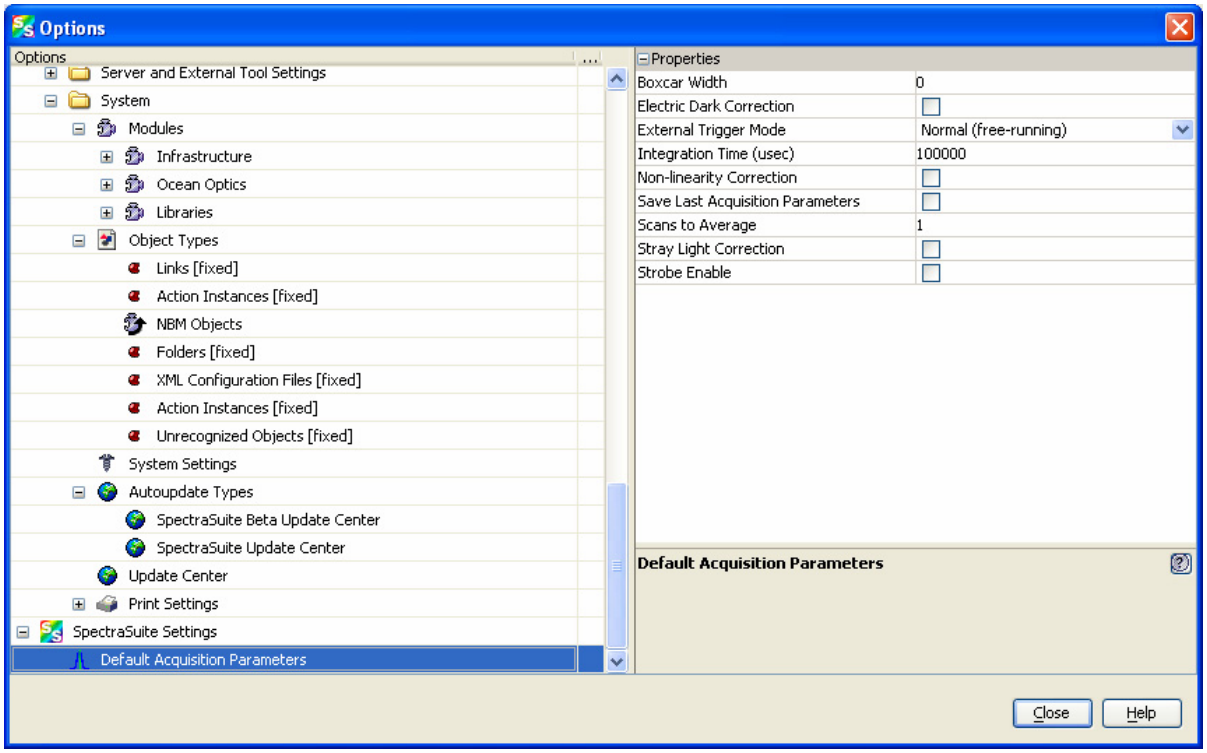
Options

Options is a powerful tool that enables you to specify the defaults for SpectraSuite parameters all in one location.



Default Acquisition Settings

You can set acquisition settings for your spectrometer(s) to persist through shutdown and restart using **Tools | Options | SpectraSuite Settings | Default Acquisition Parameters**.

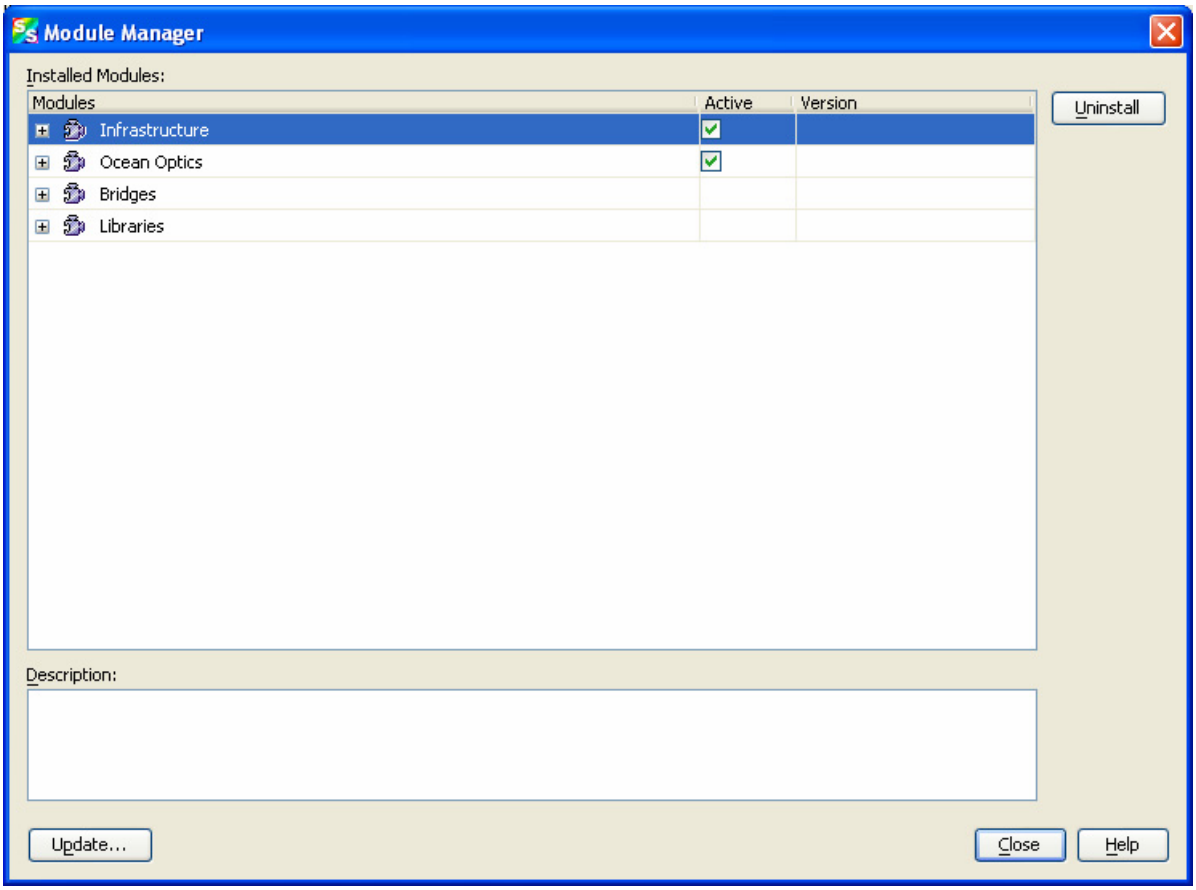


Template Manager

Future enhancement.

Module Manager

The Module Manager displays a list of installed SpectraSuite modules. You can select modules to uninstall and /or update.



Update Center

The Update Center contains a link to allow you to connect to Ocean Optic's site to download updated SpectraSuite modules. To download upgrades to SpectraSuite, you must sign up for a yearly subscription (SpectraSuite-U). Bug fixes are provides free to all SpectraSuite customers.

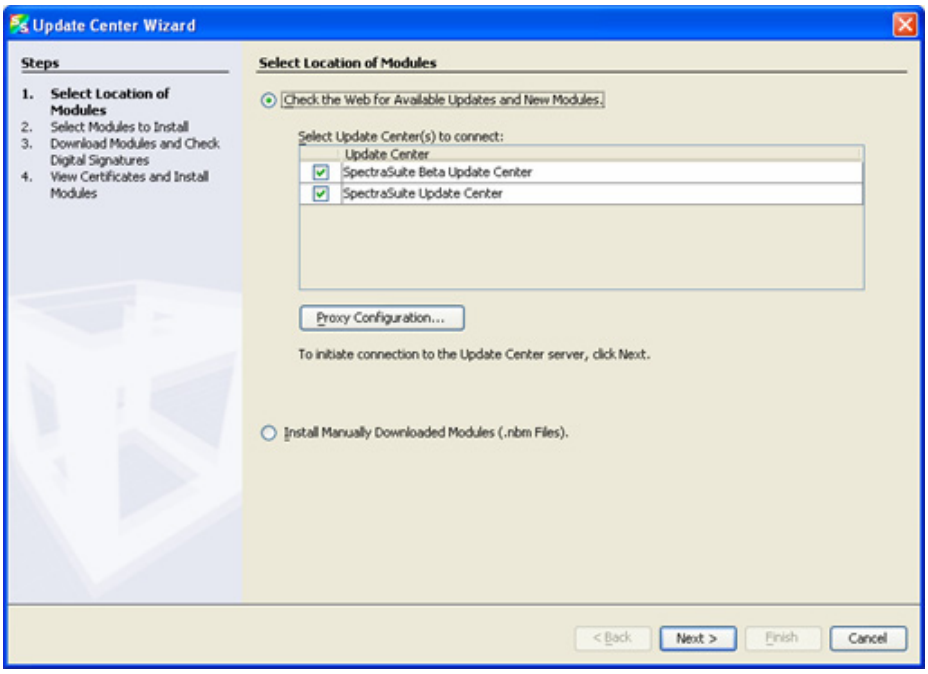
Note

If the installation computer is not connected to the Internet, download the update files on another computer and copy them to the installation computer using a USB flash drive or CD. Extract the files to a convenient location, then from within the Update Center wizard, select **Install Manually Downloaded Modules (.nbm Files)** and browse to the directory containing the downloaded files.

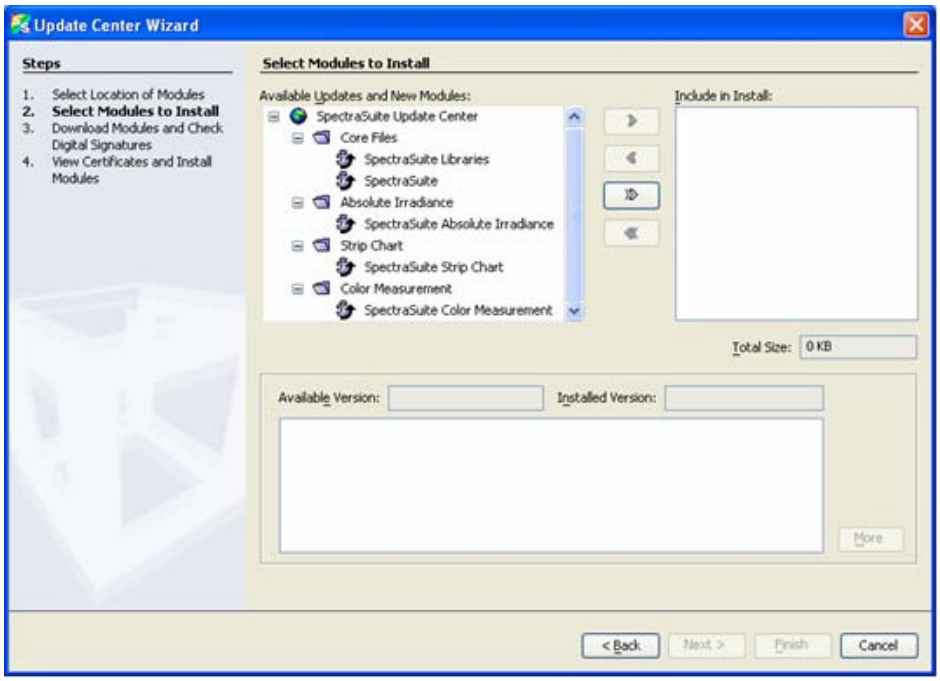
► *Procedure*

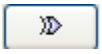
To download SpectraSuite updates,

1. Select **Tools | Update Center**. The Update Center Wizard appears.

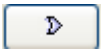

Update Center Wizard
Steps
1. Select Location of Modules
2. Select Modules to Install
3. Download Modules and Check Digital Signatures
4. View Certificates and Install Modules
Select Location of Modules
Check the Web for Available Updates and New Modules.
Select Update Center(s) to connect:
Update Center
SpectraSuite Beta Update Center
SpectraSuite Update Center
Proxy Configuration...
To initiate connection to the Update Center server, click Next.
Install Manually Downloaded Modules (.nbm Files).
< Back
Next >
Finish
Cancel

2. Click to connect to the update center. The second Update Center Wizard screen appears.



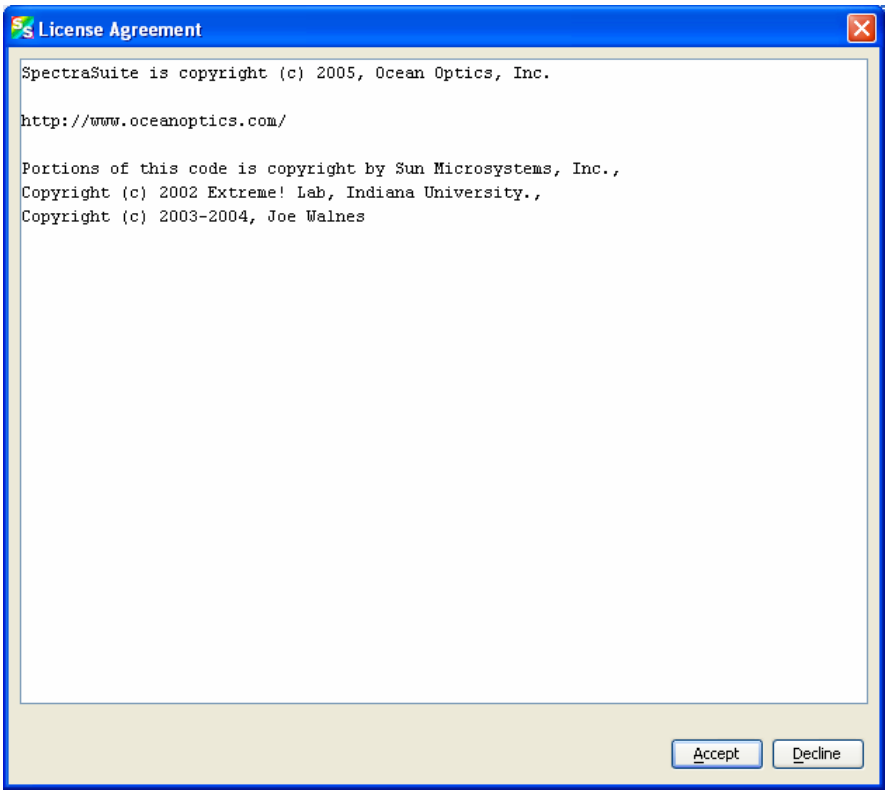
3. Click  to move the all files/modules to the **Include in Install** pane.

   Or,

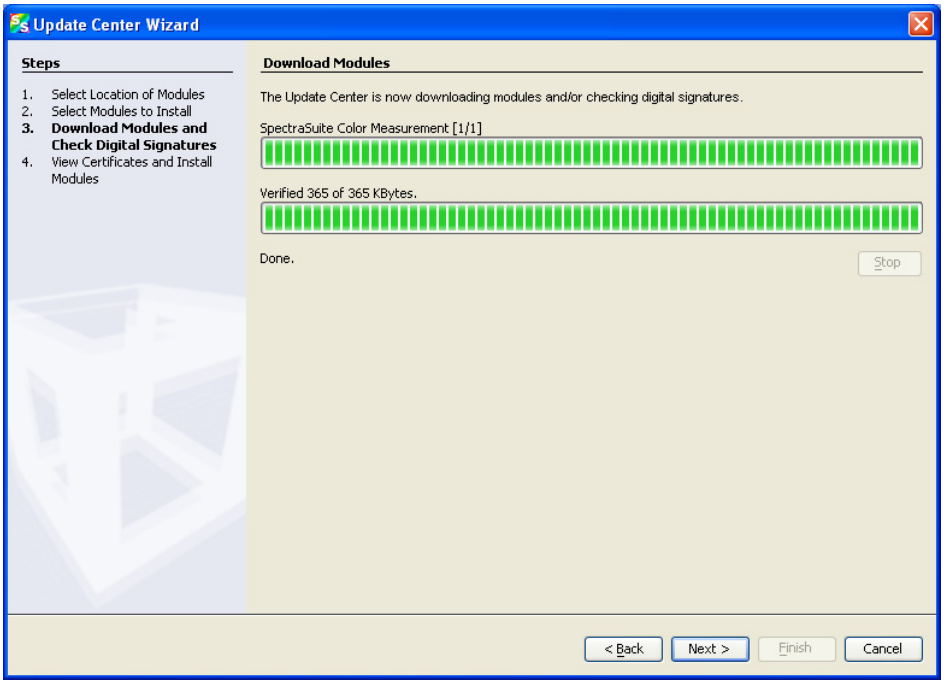
   Highlight the desired core files and/or modules to update and click  to move the selected files modules to the **Include in Install** pane. When you highlight a module or file, the size and modification date appear in the lower pane.

   Applicable version levels appear in the **Available Version** and **Installed Version** boxes.

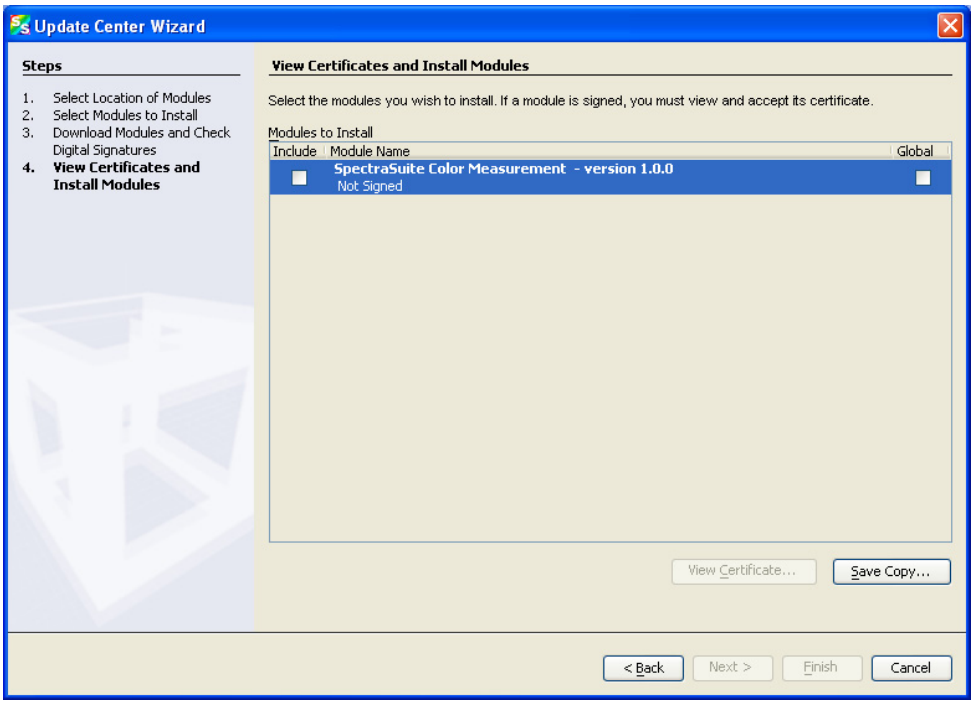
4. Click to display the SpectraSuite license agreement.


License Agreement
SpectraSuite is copyright (c) 2005, Ocean Optics, Inc.
http://www.oceanoptics.com/
Portions of this code is copyright by Sun Microsystems, Inc.,
Copyright (c) 2002 Extreme! Lab, Indiana University.,
Copyright (c) 2003-2004, Joe Walnes
Accept
Decline

5. Click to accept the license agreement and start the download. The progress of the download appears on the next screen.



6. Click Next >. The next Update Center Wizard screen appears.


Update Center Wizard
Steps
1. Select Location of Modules
2. Select Modules to Install
3. Download Modules and Check Digital Signatures
4. View Certificates and Install Modules
View Certificates and Install Modules
Select the modules you wish to install. If a module is signed, you must view and accept its certificate.
Modules to Install
Include
Module Name
Global
SpectraSuite Color Measurement - version 1.0.0
Not Signed
View Certificate...
Save Copy...
< Back
Next >
Finish
Cancel

7. Check the boxes on both sides (both Install and Global) next to the files/modules you want to install. If a module is signed, you must first view and accept its certificate. If the module isn't signed, a dialog box appears asking you to confirm that you want to install an unsigned module. Then click Finish to install the module(s).The Restart the IDE dialog box appears asking you whether you want to restart the IDE now or wait until later. If you choose to restart now, a dialog box appears asking you to confirm that you want to quit the SpectraSuite application. Once the IDE is restarted, the updates become active.

Chapter 9

Window Menu Functions

Overview

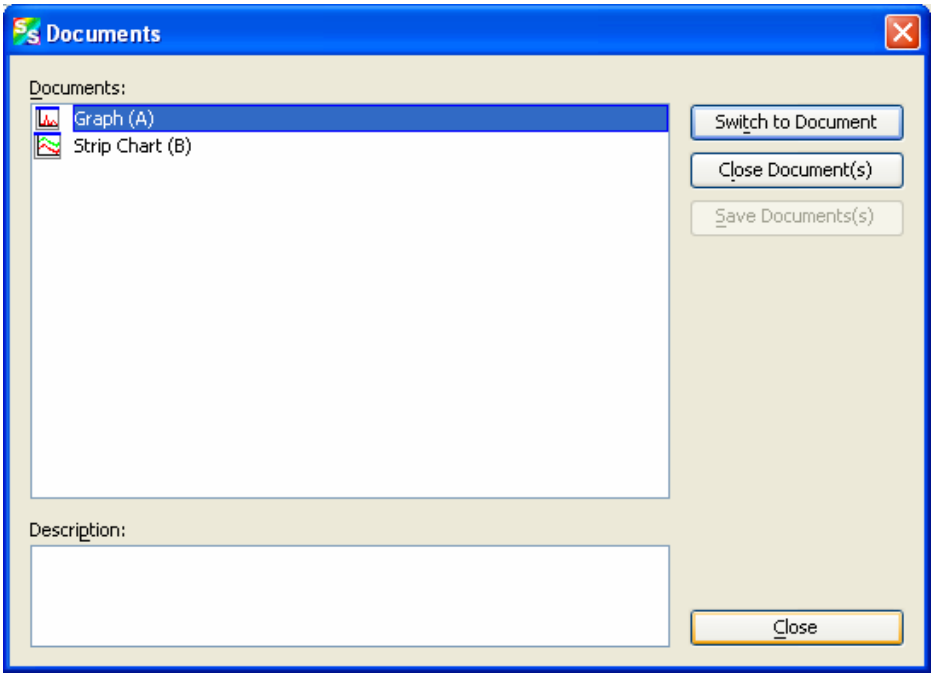
The Windows menu provides functions for manipulating the SpectraSuite graph windows.

Close All Documents

Use this function to immediately close all the SpectraSuite

Documents

Select **Window | Documents** to display the Documents dialog box. Use this dialog box to switch the SpectraSuite display to one you select, close selected document(s), or save selected document(s).

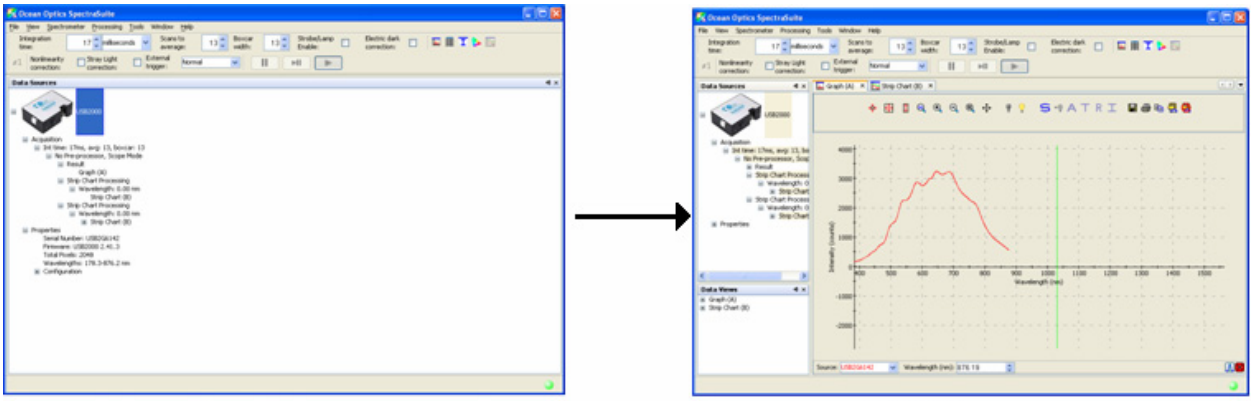


Close Window

Use this selection to close the currently selected graph window.

Maximize/Restore Window

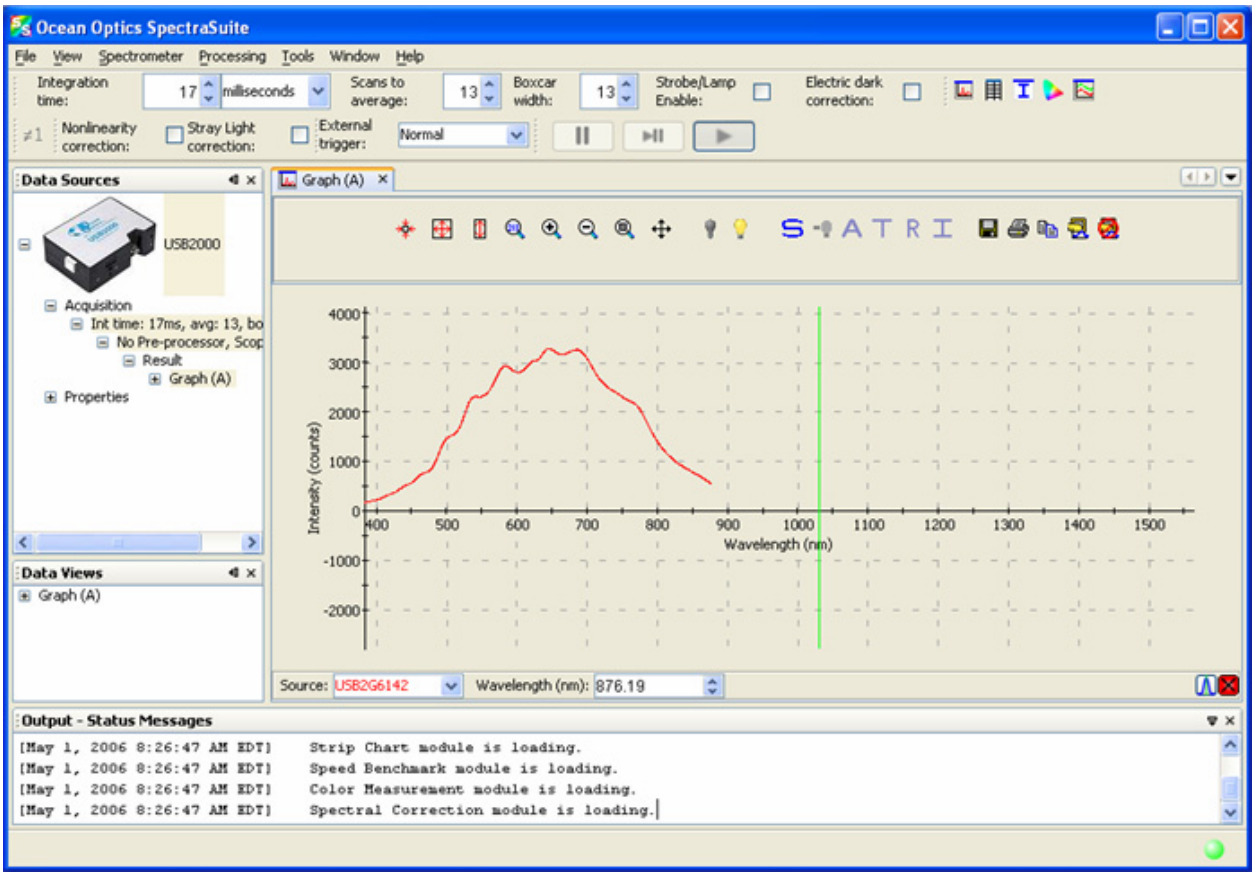
This selection toggles between maximizing the SpectraSuite currently selected SpectraSuite pane to fill the entire SpectraSuite window, and redisplaying (restoring) these panes in the window. See the example of a maximized Data Sources pane below.



Maximize Restore

Output

Select **Window | Output** to display a list of SpectraSuite status messages in a pane below the SpectraSuite window.


Ocean Optics SpectraSuite
File View Spectrometer Processing Tools Window Help
Integration time: 17 milliseconds
Scans to average: 13
Boxcar width: 13
Strobe/Lamp Enable:
Electric dark correction:
Nonlinearity correction:
Stray Light correction:
External trigger:
Normal
Data Sources
USB2000
Acquisition
Int time: 17ms, avg: 13, bo
No Pre-processor, Scop
Result
Graph (A)
Properties
Data Views
Graph (A)
Graph (A)
Intensity (counts)
Wavelength (nm)
Source: USB2G6142
Wavelength (nm): 876.19
Output - Status Messages
[May 1, 2006 8:26:47 AM EDT] Strip Chart module is loading.
[May 1, 2006 8:26:47 AM EDT] Speed Benchmark module is loading.
[May 1, 2006 8:26:47 AM EDT] Color Measurement module is loading.
[May 1, 2006 8:26:47 AM EDT] Spectral Correction module is loading.

Chapter 10

Strip Charts

Overview

SpectraSuite allows you to use Strip Charts to track processes, perform kinetic analyses, and monitor spectral events all as a function of time. The Strip Chart shows you how the value that you selected appears over time. This value can be any of the following:

One pixel (a single wavelength)

The average of a range of pixels

An integral calculated by one of three methods representing the area beneath the graph's trend line

You can acquire this data using any processing mode (transmission, absorbance, etc.).

Creating Strip Charts

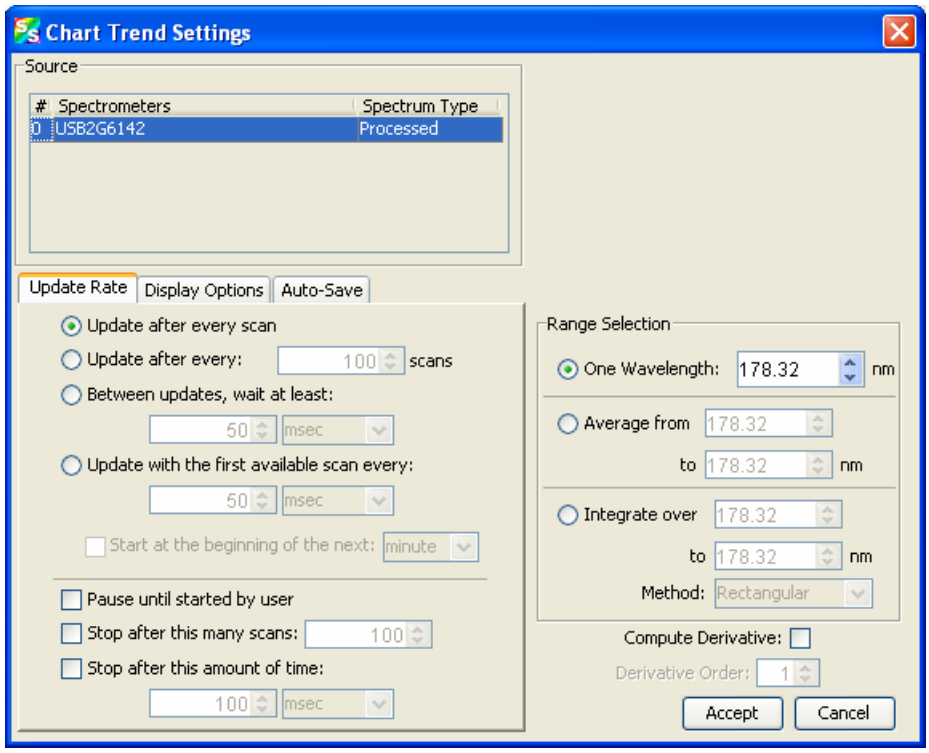
► ***Procedure***

1. Place SpectraSuite in Scope mode by clicking the Scope ( ) icon in the Experiment mode toolbar or selecting **Processing | Processing Mode | Scope** from the menu.
2. Store a reference spectrum and a dark spectrum.
3. Choose the measurement mode (absorbance, transmission, etc.).
4. Click the Strip Chart button ( )

   OR

   Select **File | New | Strip Chart** from the menu.

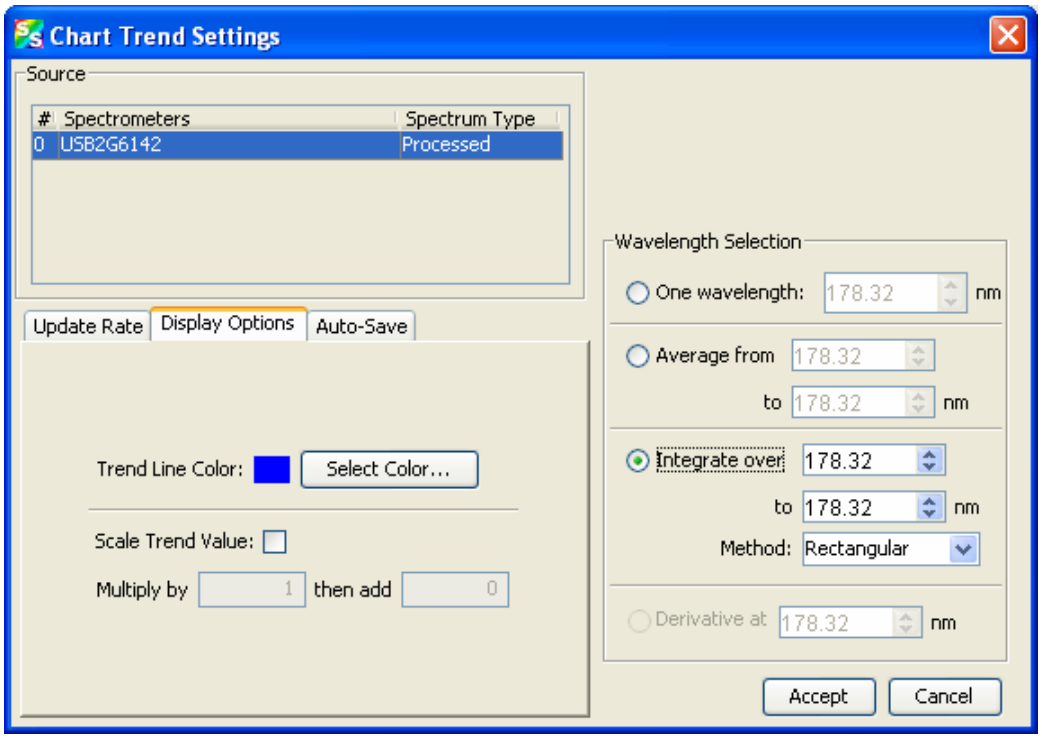
   The **Chart Trend Settings** dialog box opens with the Update Rate tab shown.



5. Enter the following data to create your Strip Chart:

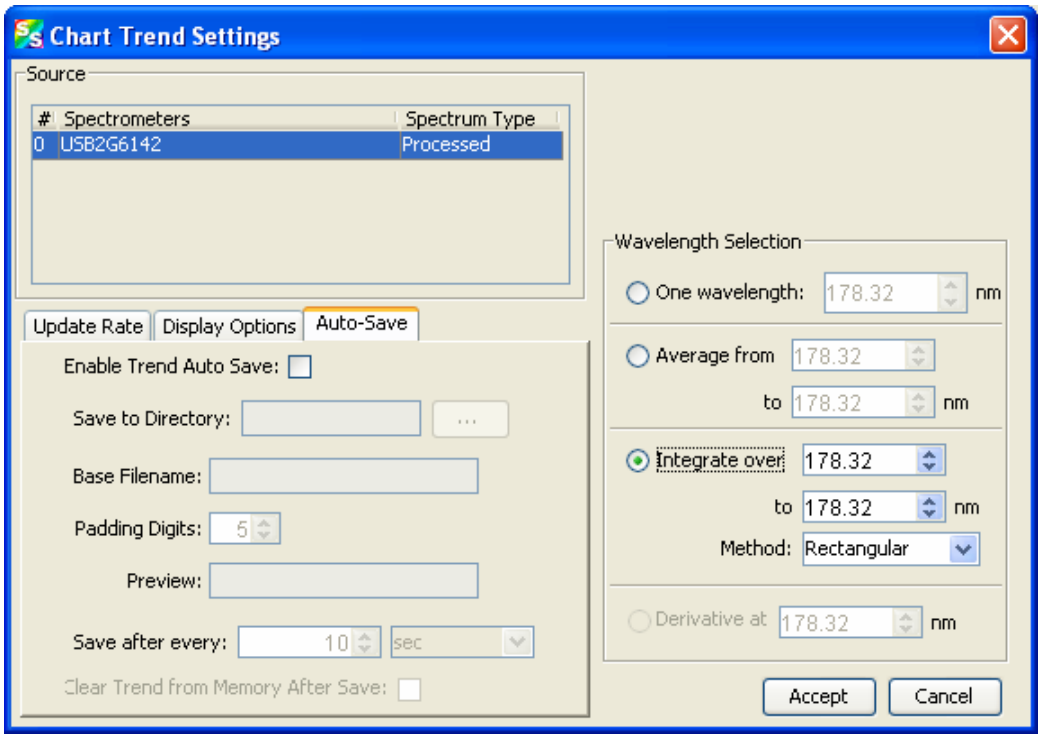
Field	Selections
Source	Select the source of the Strip Chart.
Update Rate tab: Update after every scan Update after every *x* scans Between updates, wait at least Update with the first scan every Start at the beginning of the next	Updates the strip chart: After every scan After the number of scans selected After the interval selected between updates After the first scan, then at the interval selected At the beginning of each new selected interval
Range Selection This section varies, depending on the units chosen for the x-axis (see *X-axis Units*)	Select the type of data for which you want to view the time trend from the following: One wavelength – For one pixel (used in fluorescence, for example). Select the wavelength. Average from – For a range of pixels. Select the starting and ending wavelengths. Integrate over – For the area underneath the trend line. Select the starting and ending wavelengths. Then, select the method for calculating the continuous area underneath the graph curve: Rectangular, Simpson's, or Trapezoid.

6. Click the Display Options tab.



Field	Selections
Display Options	Select a color for the graph's trend line.
Scale Trend Value	If you would like to adjust your data, enter the appropriate information in this field.

7. Click the Auto-Save tab.

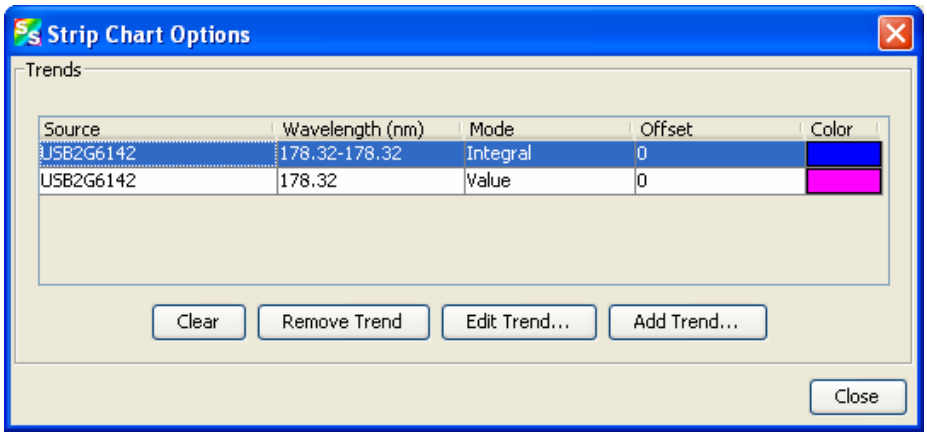


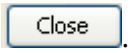
Field	Selections
Auto-Save: Enable Trend Auto-Save Save to Directory Base Filename Padding Digits Preview Save after every Clear Trend from Memory After Save	 Enables the auto-save option Enter the directory where you want to save the files Enter the filename to be used Enter the number of digits to be used when appending to a file (enter 3 to save hundreds of files, enter 4 to save thousands, etc. up to 15), for example: spectrumfile001 through spectrumfile999 if 3 is selected For future use Enter the time interval for the save. If set to 0, every scan is saved. Flushes the data from memory after each autosave to conserve memory usage.

8. Click Accept. The **Strip Chart Options** dialog box appears. **Strip Chart Options** lists all of the Strip Charts that you have created, along with the options that you have set for each one. Use this dialog box to add, edit, remove, or clear trends.

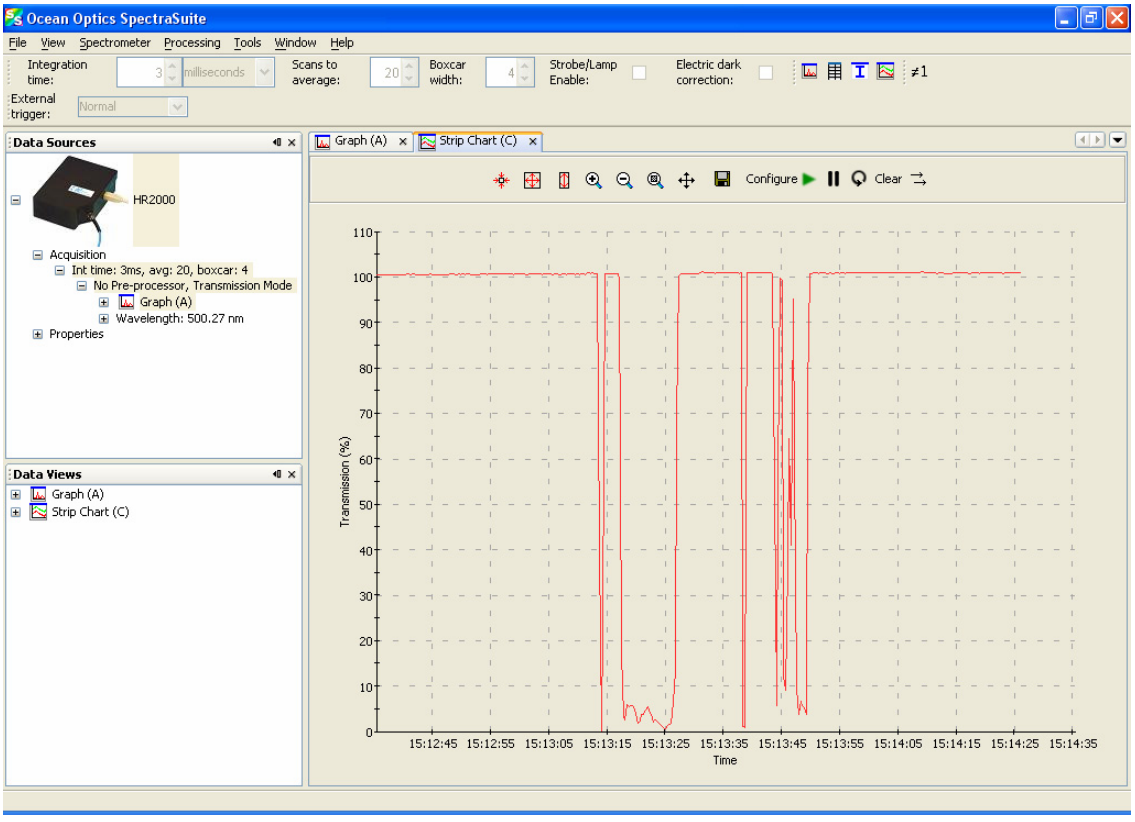
Note

Highlight the desired trend to make the **Clear**, **Remove Trend**, and **Edit Trend** buttons active.



9. Click  . The strip chart you created appears. Note the time scale along the x-axis. The y-axis in this example shows the percentage transmission for the selected pixel(s).

10. To add another trend to this graph, click .



Saving Strip Chart Data

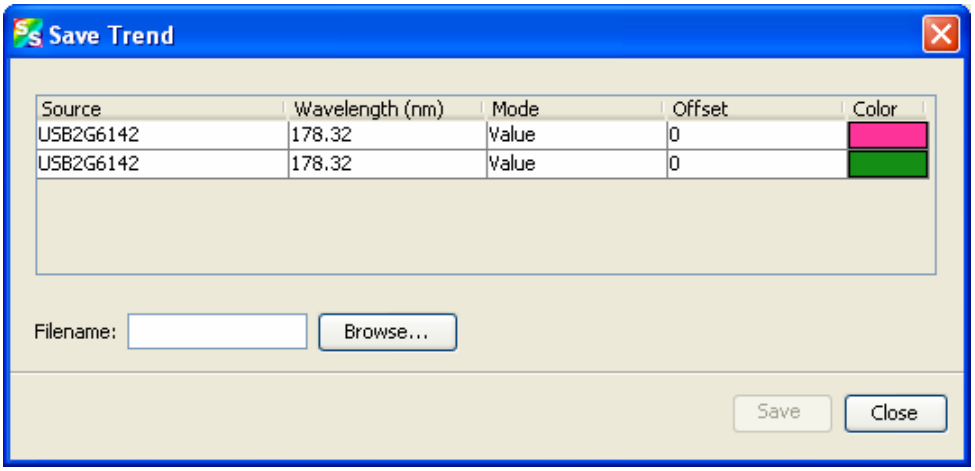
Note

See *Creating Strip Charts* for information on autosaving.

► *Procedure*

To save strip chart data:

1. From the Strip Chart graph, click . The **Save Trend** dialog box appears.



2. Select the trend to save and enter a file name. Then click Save....

Strip Chart Controls

Use the following controls to adjust the display of your strip chart.

Control	Action
▶	Resumes any strip chart trends you have paused.
⏸	Pauses all strip chart trends.
↻	Restarts any strip chart trends with a fixed length or duration (see *Creating Strip Charts*).
Clear	Clears all strip chart trends.
⇄	Automatically scrolls the strip chart graph to the newest data.

Appendix A

Experiment Tutorials

Overview

The following sections contain information on conducting sample experiments using a USB2000 Spectrometer and SpectraSuite.

For information on experiments with Ocean Optics spectrometers other than the USB2000, consult the operating instructions for your particular spectrometer model.

Preparing for Experiments

Verify that you have correctly installed SpectraSuite, installed the spectrometer, and configured the light source and other sampling optics.

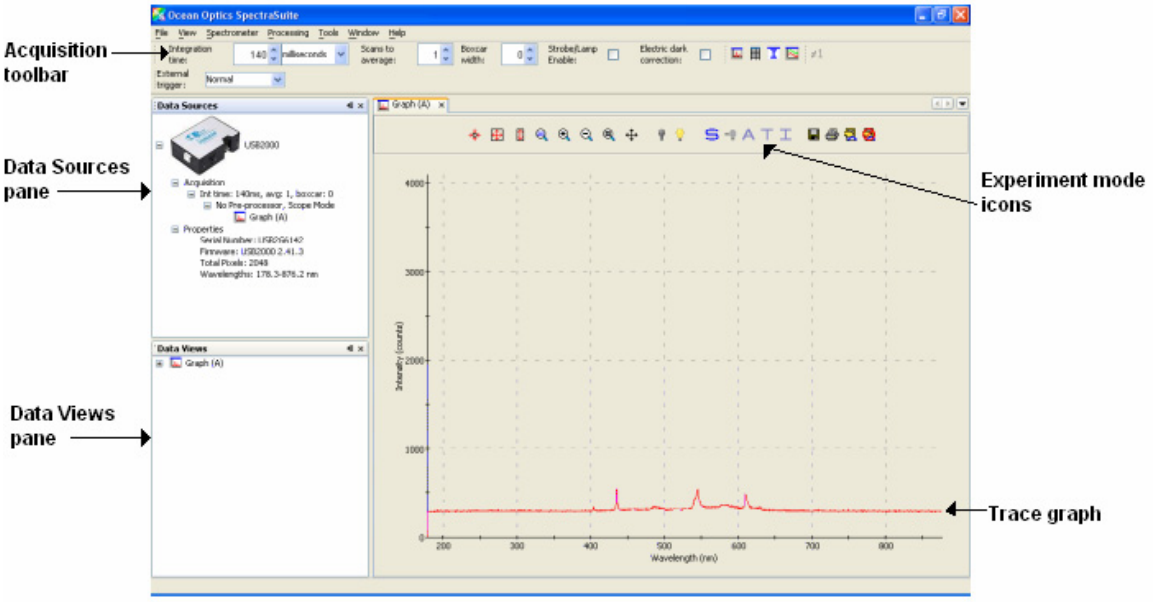
If you followed the previous steps and started SpectraSuite, the spectrometer is already acquiring data in Scope mode. Even with no light in the spectrometer, SpectraSuite should display a dynamic trace in the bottom of the graph window. If you allow light into the spectrometer, the graph trace should rise with increasing light intensity. This indicates that you correctly installed the software and hardware.

Note the spectrometer(s) that you have installed are listed in the Data Sources pane. Information for each spectrometer listed in this pane consists of the following:

Acquisition parameters that you set via the (integration time, scans-to-average, boxcar smoothing),

Whether reference and/or dark spectra have been stored, the graph (A, B, C, etc.) associated with this spectrometer that appears in the right pane (important if you have installed more than one spectrometer),

Spectrometer’s properties (serial number, firmware level, number of pixels, and wavelengths).



Once you install the hardware and software, and establish your sampling system, you are ready to take measurements.

This section details the following types of experiments:

Absorbance Experiments

Concentration Experiments

Transmission Experiments

Reflection Experiments

Irradiance Experiments

Fluorescence

The type of measurement you will take determines the configuration of the sampling optics for your system. Furthermore, your choice of reference and data analysis determines how SpectraSuite presents the results.

Note

For each measurement, you must first take a reference and dark spectrum before the experiment mode icon (A , T , I) on the toolbar becomes active. After you take a reference and a dark spectrum, you can take as many measurement scans as needed. However, if you change any sampling variable (integration time, averaging, smoothing, fiber size, etc.), you must store a new reference and dark spectrum.

Application Tips

If the signal you collect is saturating the spectrometer (intensity greater than 4000 counts), you can decrease the light level on scale in scope mode by:

Decreasing the integration time

Attenuating the light going into the spectrometer

Using a smaller diameter fiber

Using a neutral density filter with the correct optical density

If the signal you collect has too little light, you can increase the light level on scale in scope mode by:

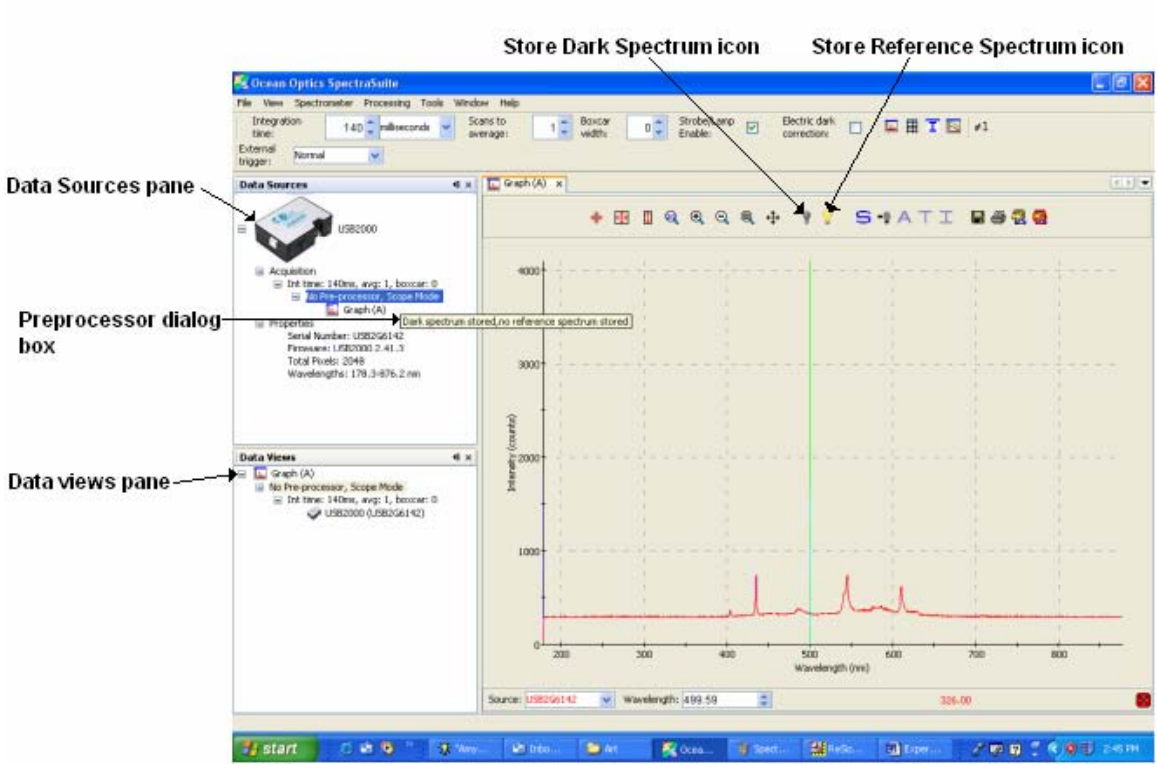
Increasing the integration time

Using a larger diameter fiber

Removing any optical filters

Taking Reference and Dark Spectra

Reference and dark spectra must be stored before collecting experiment data. If you pass the cursor over the **No-preprocessor** line in either the Data Sources or Data Views pane, a dialog box informs you whether reference and/or dark spectra have been stored.



A reference spectrum is taken when the light source is on and the there is no sample present. Click the Store Reference Spectrum icon ( ) to take a reference spectrum.

A dark spectrum is taken in the absence of light. Block the light path, uncheck the **Strobe/Lamp Enable** option on SpectraSuite's Acquisition toolbar, or turn off the lamp, and then click the Store Dark Spectrum icon ( ) to take a dark spectrum.

Absorbance Experiments

Absorbance spectra are a measure of how much light a sample absorbs. For most samples, absorbance relates linearly to the concentration of the substance. SpectraSuite calculates absorbance (A_λ) using the following equation.

$$A_\lambda = -\log_{10}\left(\frac{S_\lambda - D_\lambda}{R_\lambda - D_\lambda}\right)$$

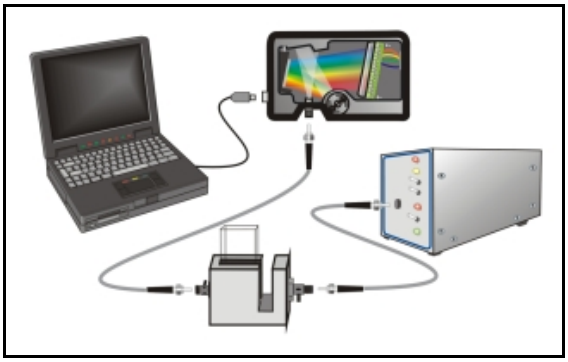
Where:

S_λ = Sample intensity at wavelength λ

D_λ = Dark intensity at wavelength λ

R_λ = Reference intensity at wavelength λ

Typical absorbance setup: The light source (far right) sends light via an input fiber into a cuvette in a cuvette holder (bottom center). The light interacts with the sample. The output fiber carries light from the sample to the spectrometer (top center) connected to the computer (far left).



Absorbance is also proportional to the concentration of the substance interacting with the light (this is known as Beer's Law). Common absorption applications include the quantification of chemical concentrations in aqueous or gaseous samples.

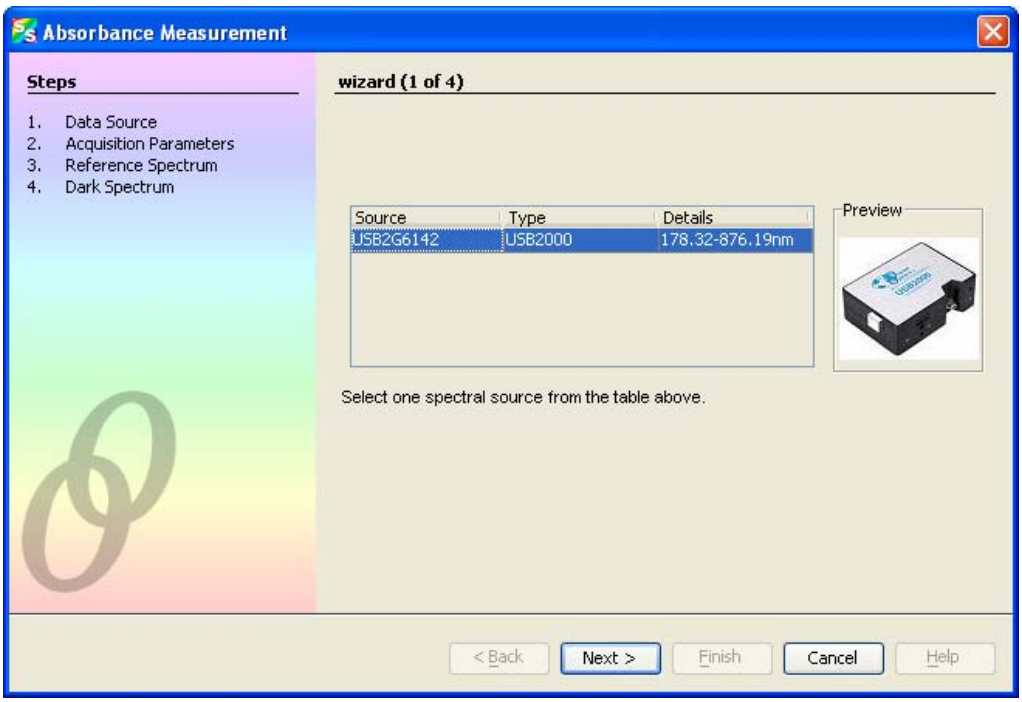
► *Procedure*

Follow the steps below to take an absorbance measurement using SpectraSuite:

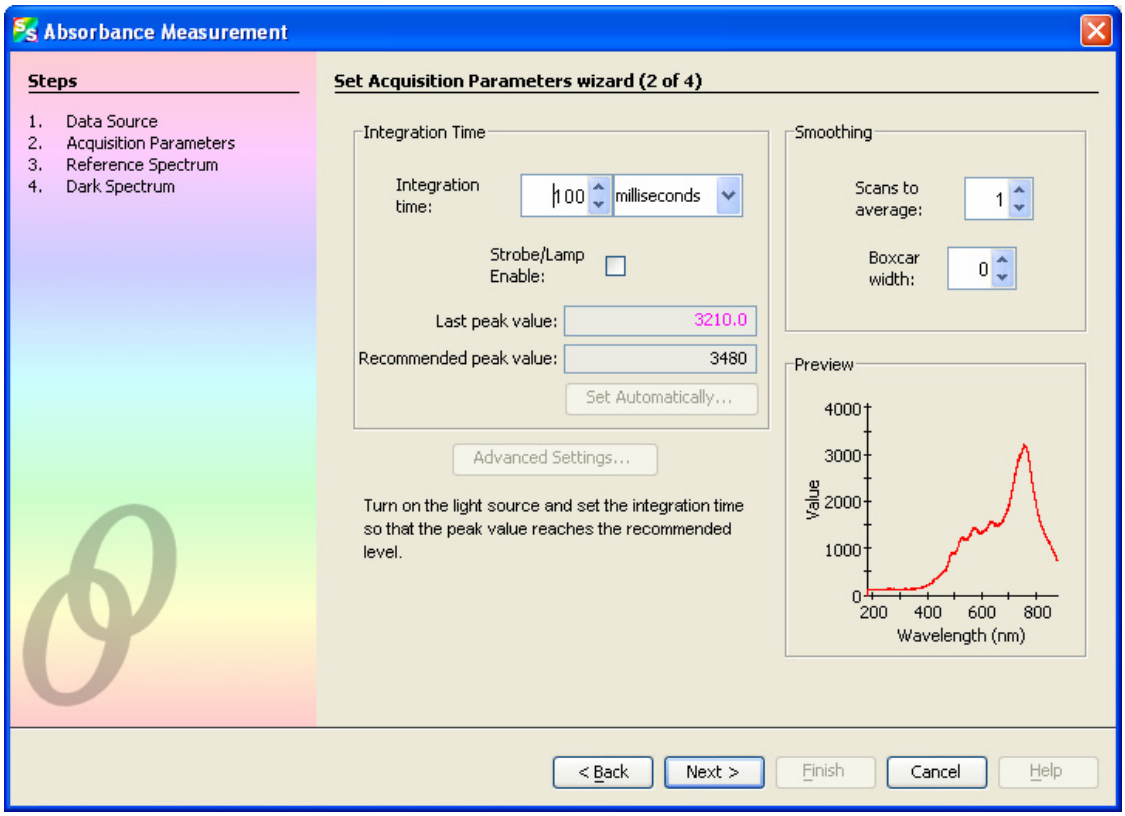
1. Place SpectraSuite in Scope mode by clicking the Scope (S) icon in the Experiment mode toolbar or selecting **Processing | Processing Mode | Scope** from the menu.

2. Ensure that the entire signal is on scale. The intensity of the reference signal's peak differs depending on the device being used. If necessary, adjust the integration time until the intensity is appropriate for your device.

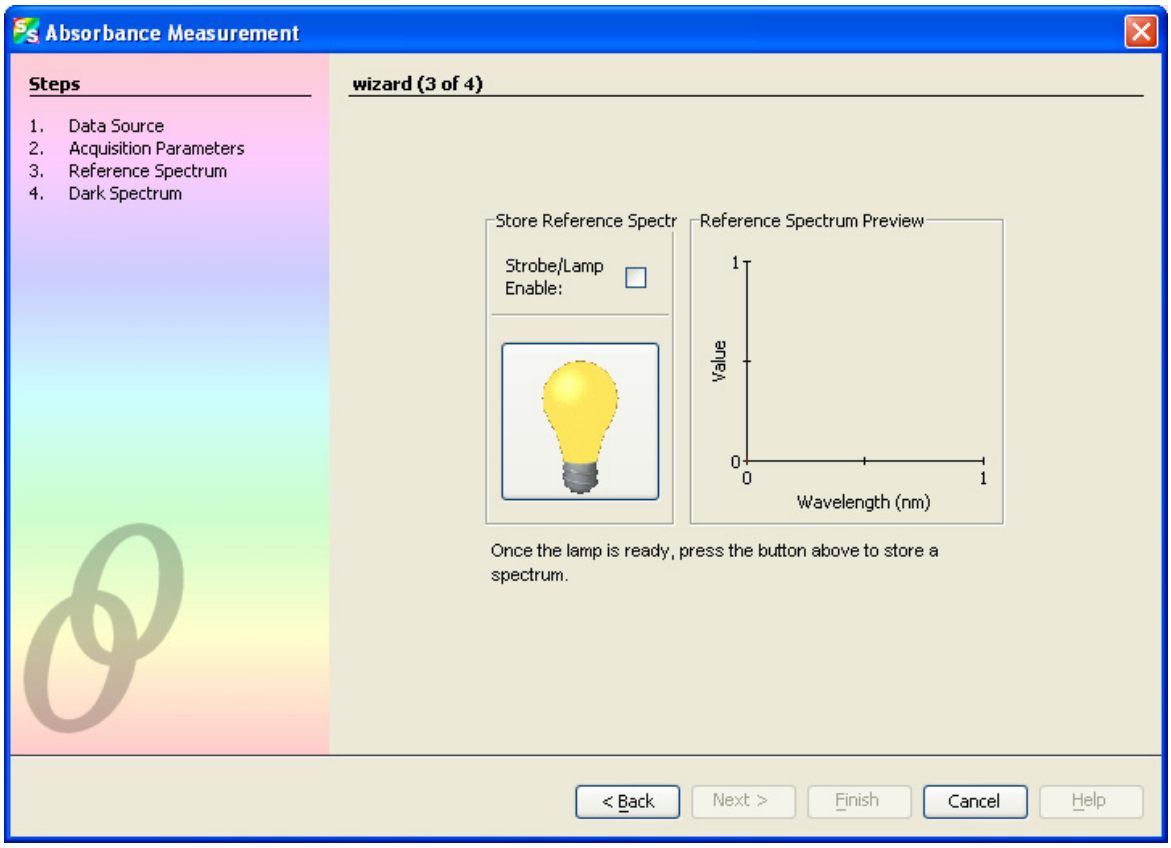
3. Select **File | New | Absorbance Measurement** from the menu or click A to start the Absorbance Measurement Wizard.



4. Select the source of your absorbance measurement and click Next >. The second page of the wizard appears.



5. Turn on your light source and set your acquisition parameters so that the peak value reaches the recommended level. Then click Next >. The third page of the wizard appears.



6. If you have not already done so, place a sample of the solvent into a cuvette to take a reference spectrum. You must take a reference spectrum before measuring absorbance.

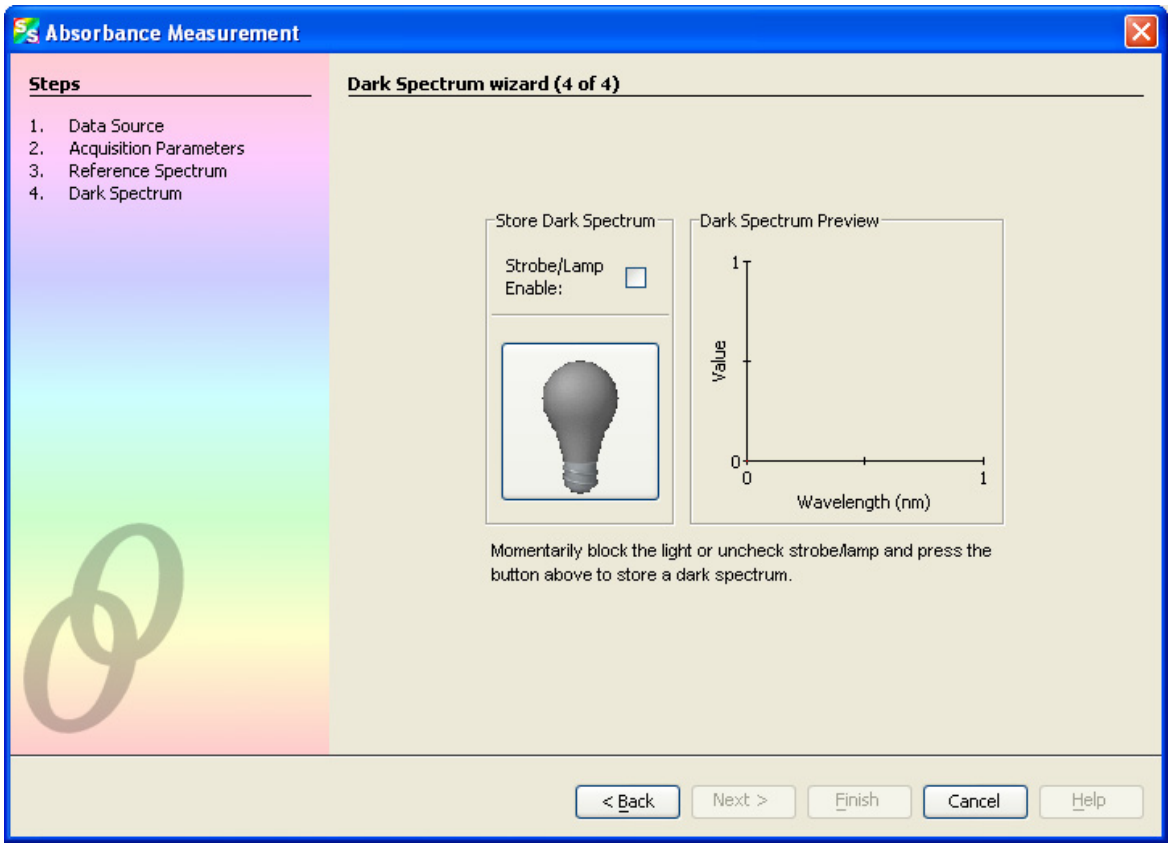
Note

Do not put the sample itself in the path when taking a reference spectrum, only the solvent.

---

7. Click the Store Reference Spectrum ( ) icon on the screen. This command merely stores a reference spectrum in memory. You must click the Save Spectra ( ) icon on the toolbar or select **File | Save | Save Spectra Collection** from the menu bar to permanently save the reference spectrum to disk.

   Then click Next >. The fourth page of the wizard appears.



8. Block the light path to the spectrometer, uncheck the **Strobe/Lamp Enable** box, or turn the light source off. Then, take a dark spectrum by clicking . You must take a dark spectrum before measuring absorbance.

   This command merely stores a dark spectrum in memory. You must click the Save Spectra ( ) icon on the toolbar or select **File | Save | Save Spectra Collection** from the menu bar to permanently save the spectrum to disk.

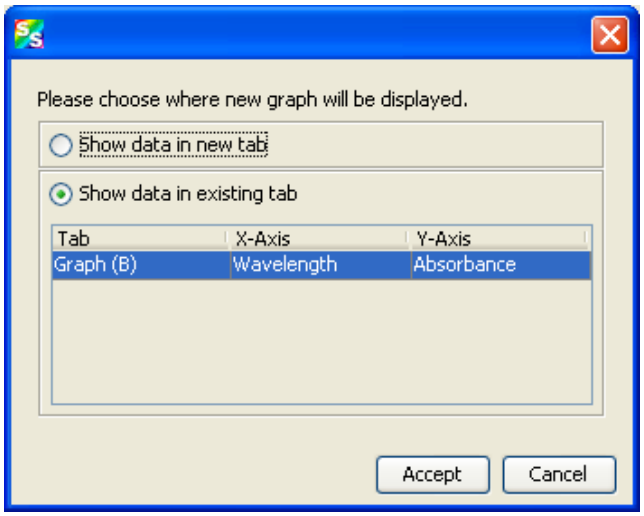
Note

If possible, do not turn off the light source when taking a dark spectrum. If you must turn off your light source to store a dark spectrum, allow enough time for the lamp to warm up again before continuing your experiment. After the lamp warms up again, store a new reference.

---

9. Put the sample in place and ensure that the light path is clear. Then, click .

   If you have already taken one or more absorbance measurements, a dialog box appears asking you to specify whether to display the new data in a new graph, or on the existing graph.



Note the following changes on the screen:

- The experiment mode listed in the Data Sources and Data Views panes changes to **Absorbance Mode**.
- The units listed on the Graph pane changes to **Absorbance (OD)**.

10. To permanently save the spectrum to disk, click the Save Spectra ( ) icon on the toolbar.

Note

If you change any sampling variable (integration time, averaging, smoothing, fiber size, etc.), you must store a new reference and dark spectrum.

Concentration Experiments

To discover the unknown concentration of a substance in a solution, you must first take spectral scans of a series of solutions with different known concentrations of the same substance. You begin this process by taking an absorbance spectrum of the solution with the highest known concentration.

While going through the wizard, when asked to store a reference spectrum, put a cuvette full of your solvent in the spectrometer's cuvette holder.

There are three methods you can use to calculate the concentration of a sample:

Using Beer's Law (see *Calculating Concentration Using Beer's Law*)

Calibrating from a solution of known concentration (see *Calibrating from Solutions of Known Concentration*)

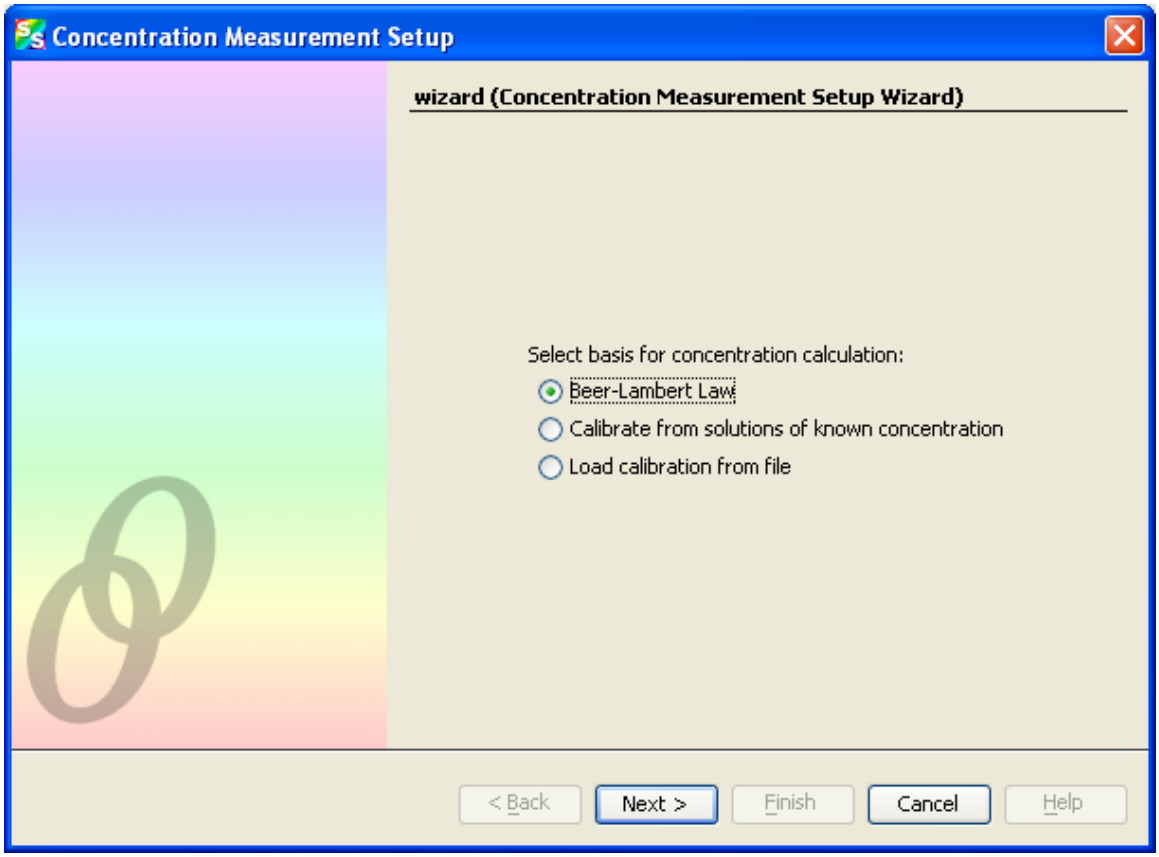
Loading a previously stored calibration from a file (see *Loading Calibration from an Existing File*)

The Concentration Measurement Setup Wizard allows you to choose one of these three methods.

Before measuring concentration, you must first take an absorbance measurement (see *Absorbance Experiments* for instructions).

► *Procedure*

1. Select **File | New | Concentration Experiment** from the menu to open the Concentration Measurement Setup Wizard.

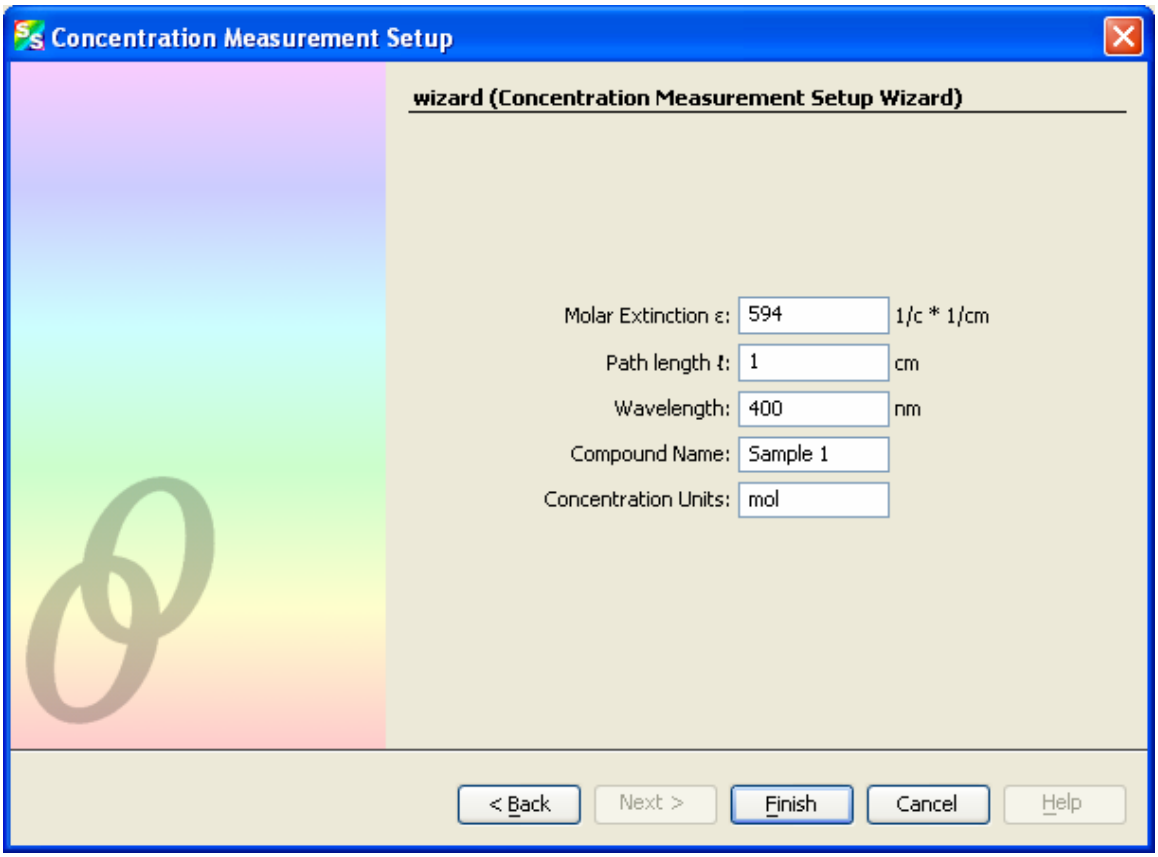


2. Select the basis for the concentration calculation.

Calculating Concentration Using Beer's Law

3. Select Beer-Lambert Law to specify the molar extinction constant ε and a wavelength. Then, Click Next >.

   The following window appears:

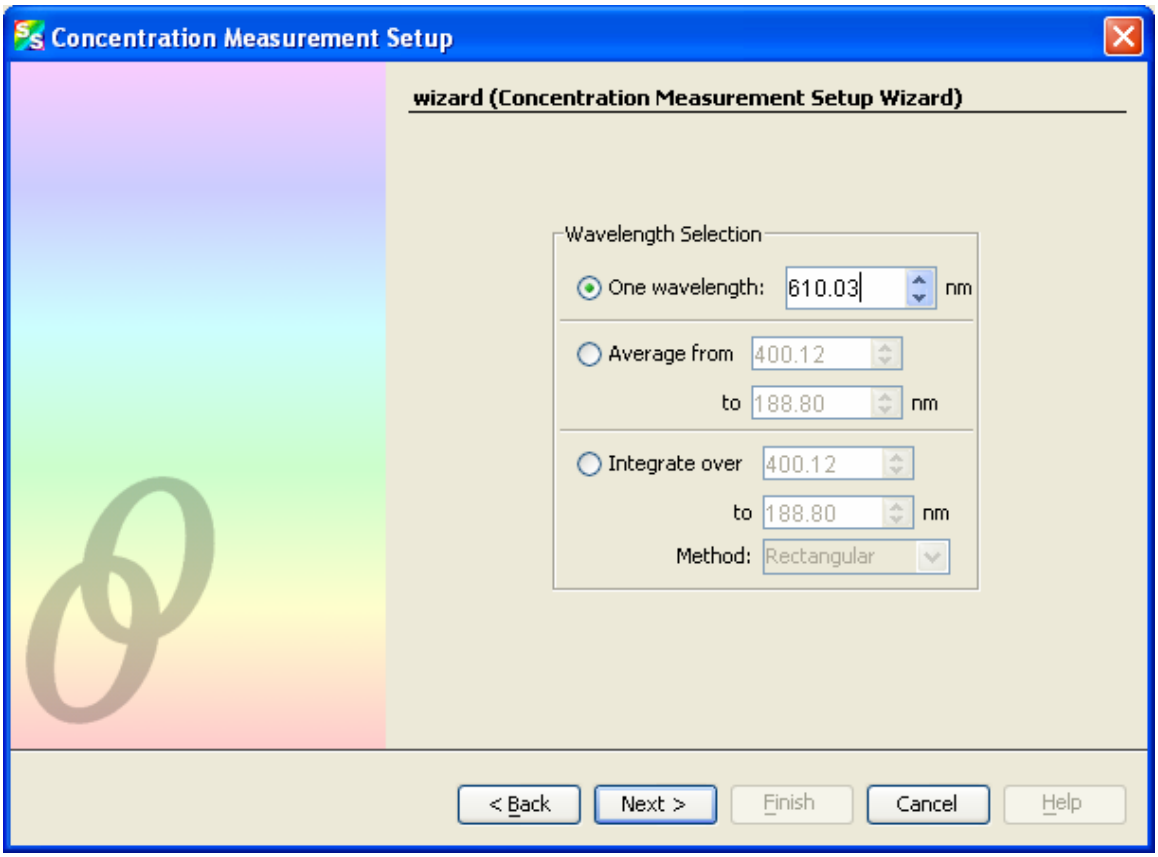


4. Fill in the fields according to the constants appropriate for your sample. The **Compound Name** and **Concentration Units** can be set to anything, and are simply provided for reference. Click Finish when done.

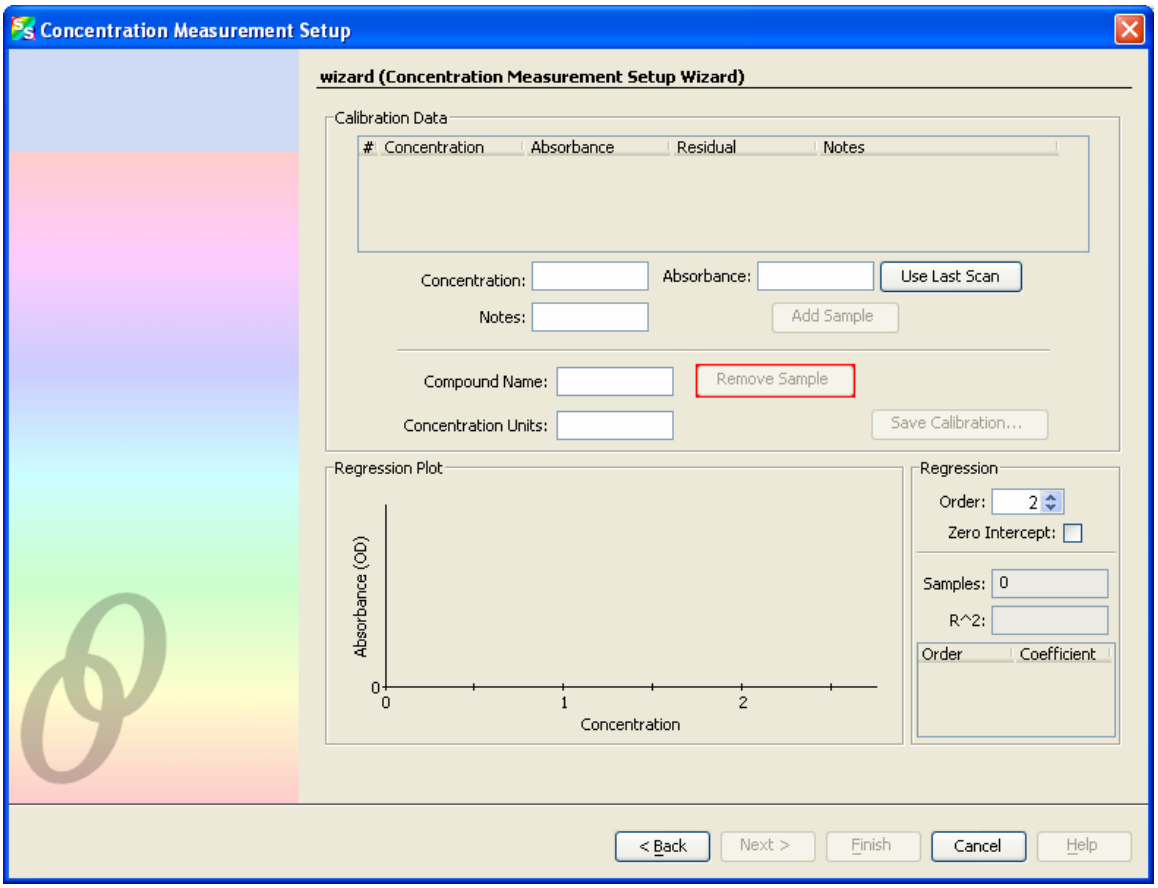
Calibrating from Solutions of Known Concentration

a. Insert a sample for which the concentration is known into the spectrometer.

b. Select **Calibrate from solutions of known concentration**, insert samples into the spectrometer for which you know the concentration and use that as a basis for computing the concentration of the unknowns. Then, click Next >. The following window appears:



c. Choose a single wavelength where the absorbance of your compound is greatest. You can also choose an average or integral over a range of wavelengths, which may provide a more robust calibration, since it is not as reliant on the behavior of the compound at one wavelength. Then click Next >. The following window appears:

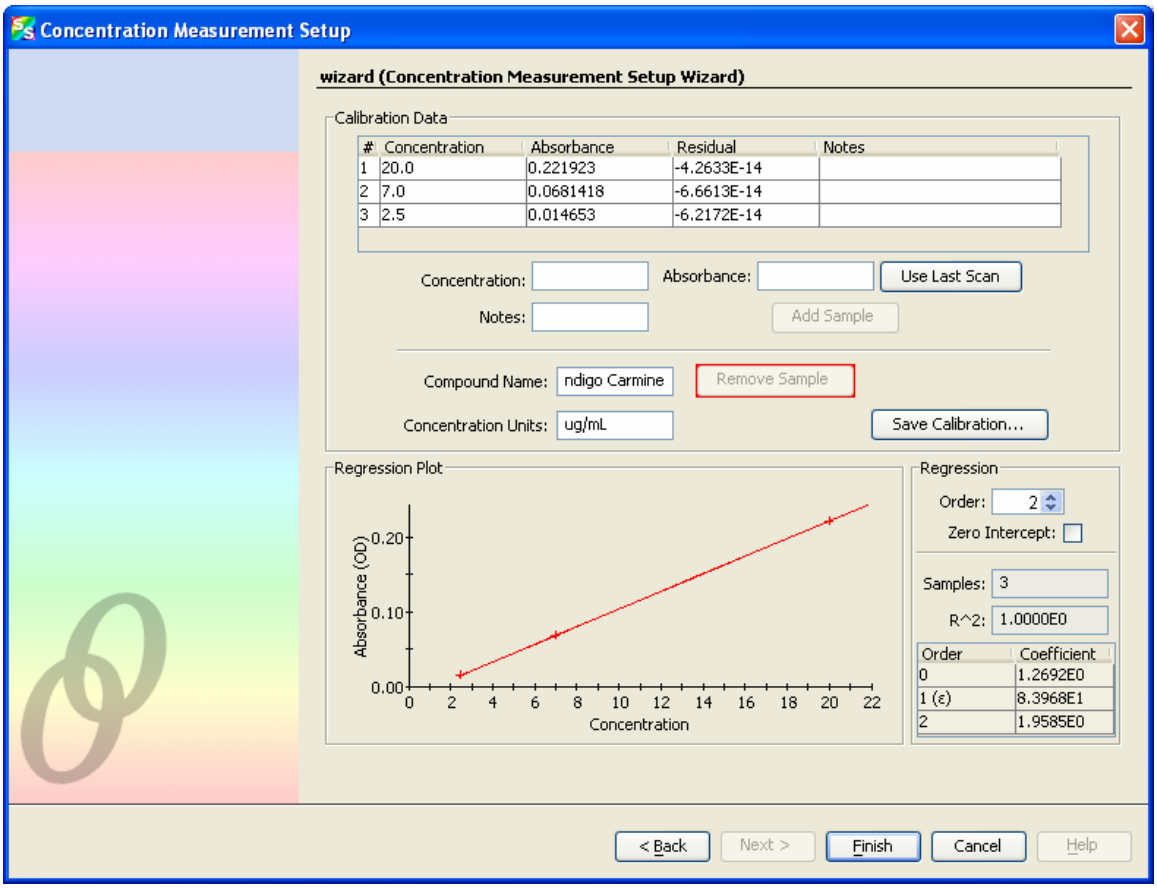


d. If desired, enter the name and concentration units for their compound in the indicated fields (this step is optional).

e. To generate a calibration, enter a known concentration in the **Concentration** field, and either manually enter the corresponding **Absorbance** or place the corresponding cuvette into the cuvette holder and click **Use Last Scan** to measure the absorbance directly. Use **Notes** to enter any comments.

f. Click **Add Sample** to log the concentration vs. absorbance point. It will appear on the Regression plot in the bottom of the window, and in the table at the top.

g. After entering a few points, a regression line will be computed through the concentration points. This indicates that sufficient points have been sampled for concentrations to be estimated from unknowns.



5. Enter options for how the regression is computed in the lower-right corner of the window:

   - **Order** – Set the regression order to **1** (straight line fit) or **2** (second order polynomial fit).
   - **Zero Intercept** – You can force the regression line to pass through the origin (that is, zero concentration and absorbance) by checking this box.

     For a first order fit, at least two data points are necessary. For a second order fit, three points are necessary. If **Zero Intercept** is selected, then only one point is required for a first order fit and two points for a second order fit.

     In general, more data points result in a better estimation of the concentration of an unknown. It is recommended that as many calibration points be sampled in this way as is practical. Also, allow your reference lamp to stabilize before attempting a calibration with many points, as any drift in the lamp's emission will introduce error into these samples.

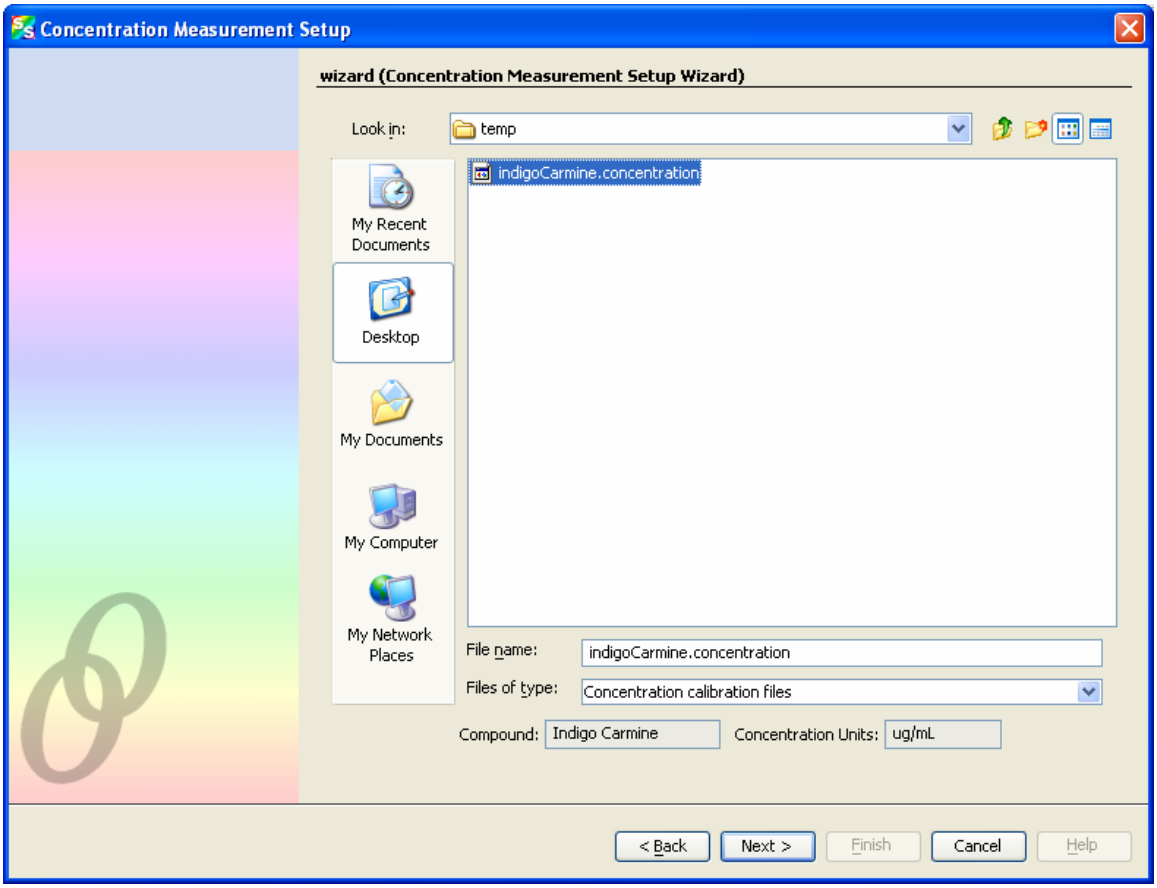
     The quality of the regression is shown in the lower right as an **R^2** value, where 1.0 is a perfect fit (lower numbers indicate a poorer fit). The residual value for each point is also shown in the table at the top of the window; this indicates the difference between the known concentration for a sampled absorbance and the estimated concentration using the regression. In the ideal case, this value will approach zero. Note that very small values (on the order of 10-12 or smaller) are normal even for a good fit; this is due to a rounding error and should have no discernable effect on solution quality.

6. At any time, you can select a sample from the table at the top of the window and click **Remove Sample** to discard the point. Once enough points exist to compute a regression, the Save Calibration... will be enabled to allow the current set of samples to be saved to disk for later retrieval.

7. Click Finish when you have entered enough points to generate a regression line.

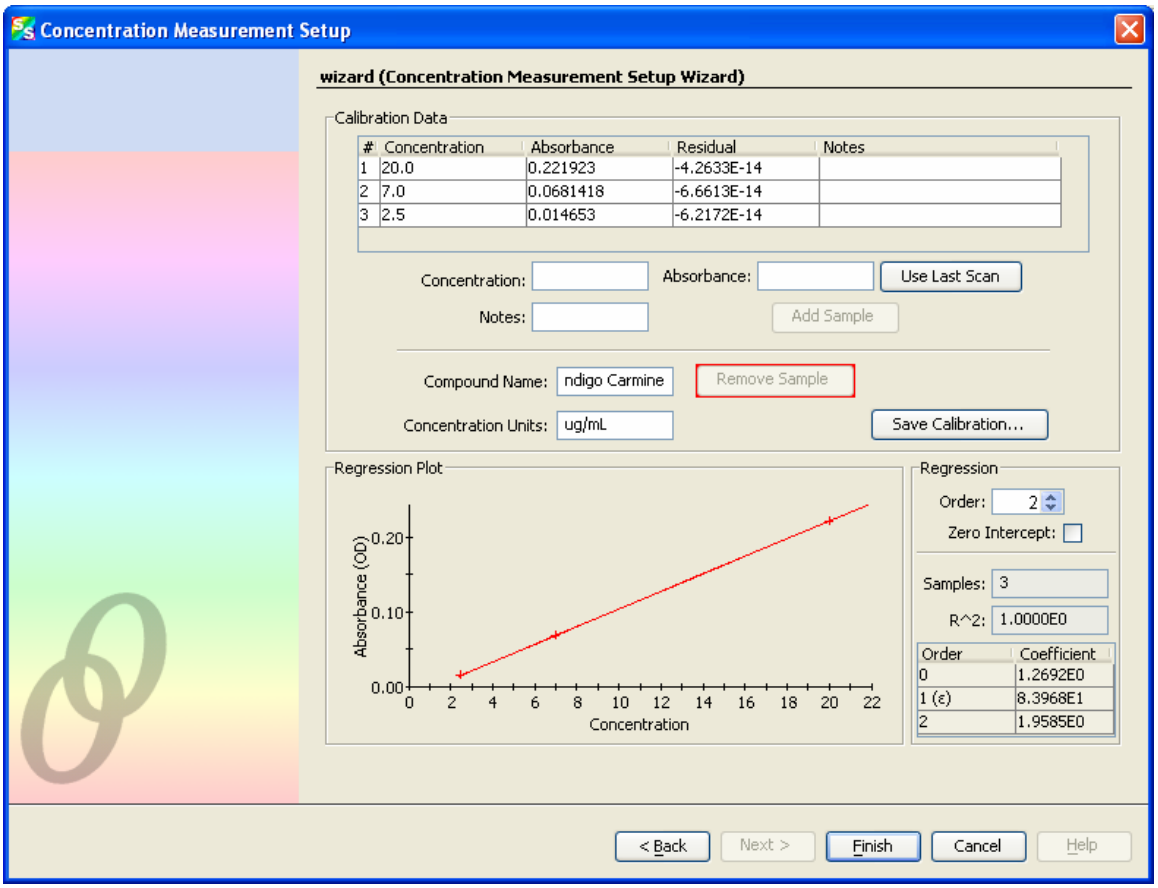
Loading Calibration from an Existing File

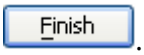
a. Select **Load calibration from file** to recall a calibration from known solutions that was performed previously. The following window appears (the example below is in Windows XP format):

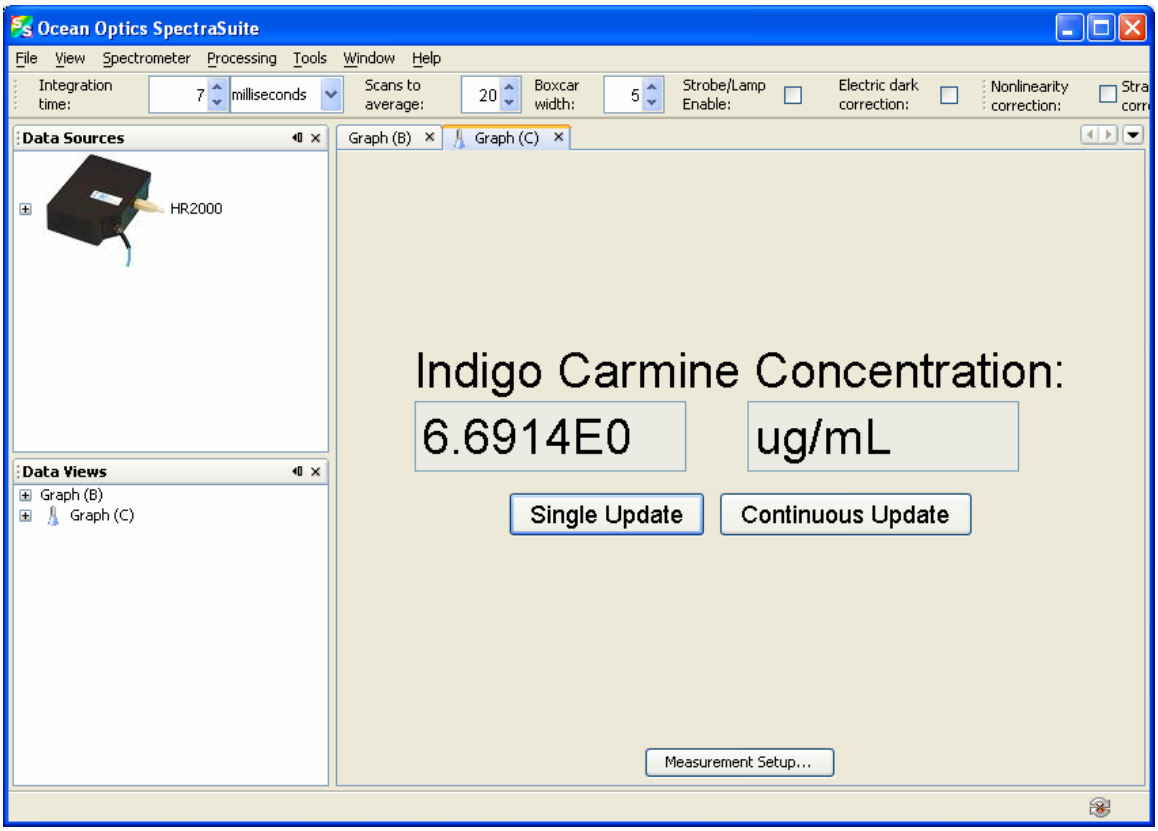


b. Select a file that was previously saved with Save Calibration... in the **Calibrating from Solutions of Known Concentration** wizard (see *Calibrating from Solutions of Known Concentration*, Step h.). When an appropriate file is selected, the name of the compound and concentration units appear near the bottom of the window.

c. Click Next >. The resulting window is the same as if you had just entered those values from a known concentration:



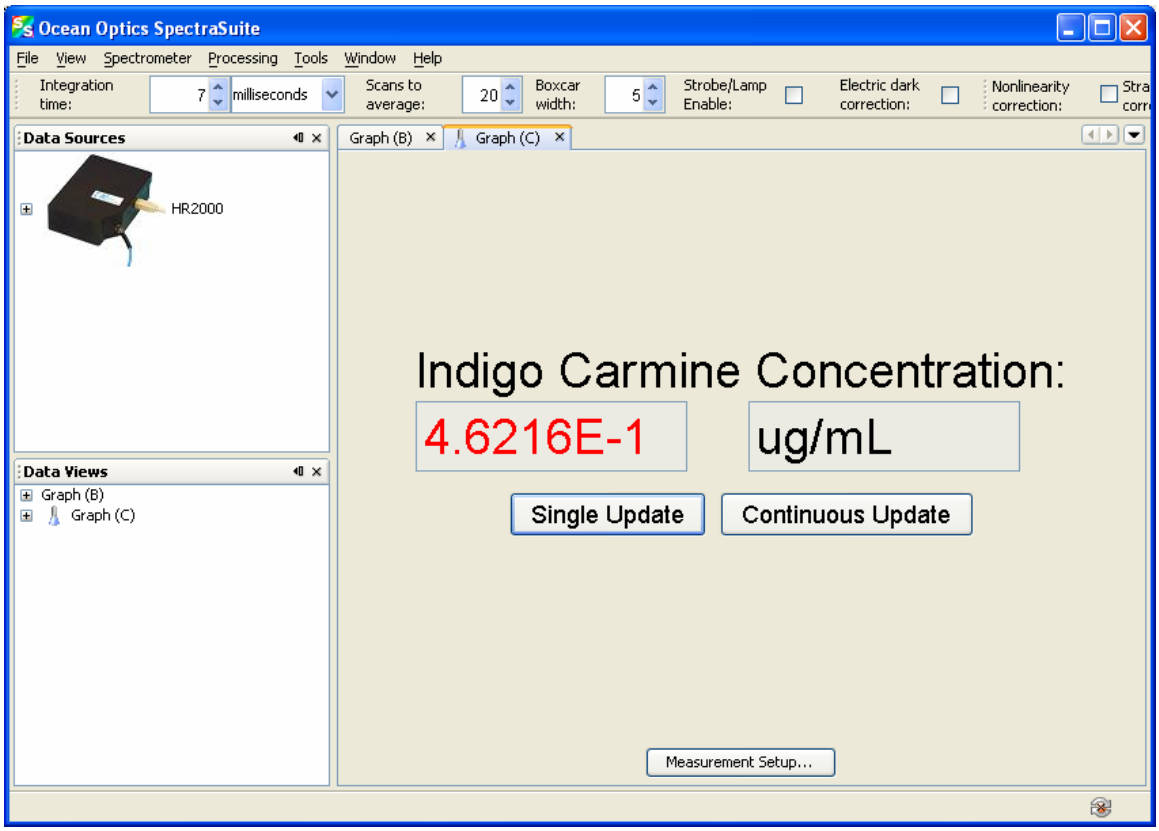
3. When the concentration of the sample has been calculated using one of the three available methods, click  . The Concentration window appears:



4. By default, the window will not update on its own. Perform a single scan by clicking Single Update (for instance, after inserting each cuvette of unknown concentration). Click Continuous Update if you want the values to update as quickly as possible.

   Note the following on this window:

   - The name of the compound and the units you provided are shown.
   - The numeric value for the concentration appears in black if the calculation was within the bounds of the measurement setup. If you calculated the concentration using the Beer-Lambert law, the concentration appears in black for any positive measured absorbance. If you calculated the concentration using known samples, the concentration will appear in black only if the measured absorbance is within the range of absorbance sampled by the user. If a sample is introduced that falls outside of this range, the concentration will appear in red to indicate that it is out-of-bounds and may not be accurate, as shown in the following example:



At any time, you can click to reopen the setup wizard and change the parameters for the concentration measurement.

Transmission Experiments

Transmission is the percentage of energy passing through a sample relative to the amount that passes through the reference. Transmission mode can also display the portion of light *reflected* from a sample, since transmission and reflection measurements use the same mathematical calculations. We express transmission as a percentage ($\%T_\lambda$) relative to a standard substance (such as air). SpectraSuite calculates $\%T_\lambda$ (or $\%R_\lambda$) with the following equation.

$$\%T_\lambda = \frac{S_\lambda - D_\lambda}{R_\lambda - D_\lambda} \times 100\%$$

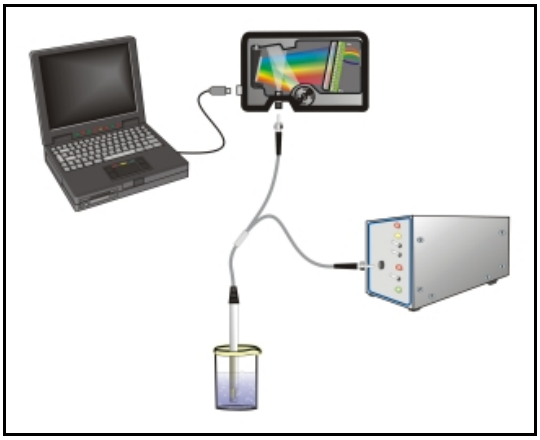
Where:

S_λ = Sample intensity at wavelength λ

D_λ = Dark intensity at wavelength λ

R_λ = Reference intensity at wavelength λ

Typical transmission setup: The light source (far right) sends light via the input leg of a transmission probe into a container (bottom center). The light interacts with the sample. The output leg of the transmission probe carries the information to the spectrometer (top center), which transmits the information to the computer (far left).



Common transmission applications include measuring light through solutions, optical filters, optical coatings, and other optical elements (such as lenses and fibers).

► *Procedure*

Perform the following steps to take a transmission measurement using SpectraSuite:

1. Place SpectraSuite in Scope mode by clicking the Scope ( ) icon in the Experiment mode toolbar or selecting **Processing | Processing Mode | Scope** from the menu.

2. Ensure that the entire signal is on scale. The intensity of the reference signal's peak differs depending on the device being used. If necessary, adjust the integration time until the intensity is appropriate for your device.

3. If you have not already done so, place a sample of the solvent into a cuvette and take a reference spectrum. You must take a reference spectrum before measuring transmission.

Note

Do not put the sample itself in the path when taking a reference spectrum, only the solvent.

Click the Store Reference Spectrum ( ) icon on the toolbar or by select **File | Store | Store Reference Spectrum** from the menu bar to store the reference. This command merely stores a reference spectrum in memory. You must click the Save Spectra ( ) icon on the toolbar to permanently save the reference spectrum to disk.

4. If you have not already done so, store a dark spectrum reading. To do this, either block the light path to the spectrometer, uncheck the **Strobe/Lamp Enable** box in the Acquisition toolbar, or turn the light source off. Then, take a dark spectrum by clicking the Store Dark Spectrum ( ) icon on the toolbar or by selecting **File | Store | Store Dark Spectrum** from the menu bar. This command merely stores a dark spectrum in memory. You must click the Save Spectra ( ) icon on the toolbar or select **File | Save | Save Spectra Collection** from the menu bar to permanently save the spectrum to disk.

Note

If possible, do not turn off the light source when taking a dark spectrum. If you must turn off your light source to store a dark spectrum, allow enough time for the lamp to warm up again before continuing your experiment.

You must take a dark spectrum before measuring transmission.

5. Put the sample in place and ensure that the light path is clear. Then, take a transmission measurement by clicking on the Transmission ( ) icon on the toolbar or selecting **Processing | Processing Mode | Transmission** from the menu. Note the following changes on the screen:

- The experiment mode listed in the Data Sources and Data Views panes changes to **Transmission Mode**.
- The units listed on the Graph pane changes to **Transmission (%)**.

6. To permanently save the spectrum to disk, click the Save Spectra ( ) icon on the toolbar or select **File | Save | Save Spectra Collection** from the menu bar.

Note

If you change any sampling variable (integration time, averaging, smoothing, fiber size, etc.), you must store a new reference and dark spectrum.

Reflection Experiments

Reflection is the return of radiation by a surface, without a change in wavelength. Reflection can be:

Specular (the angle of incidence is equal to the angle of reflection)

Diffuse (the angle of incidence is not equal to the angle of reflection)

Every surface returns both specular and diffuse reflections. Some surfaces may return mostly specular reflection, while others may return mostly diffuse reflection. Specular reflection increases proportionately with the amount of gloss on a surface.

Reflection is expressed as a percentage (%R_λ) relative to the reflection from a standard reference substance:

$$\%R_\lambda = \frac{S_\lambda - D_\lambda}{R_\lambda - D_\lambda} \times 100\%$$

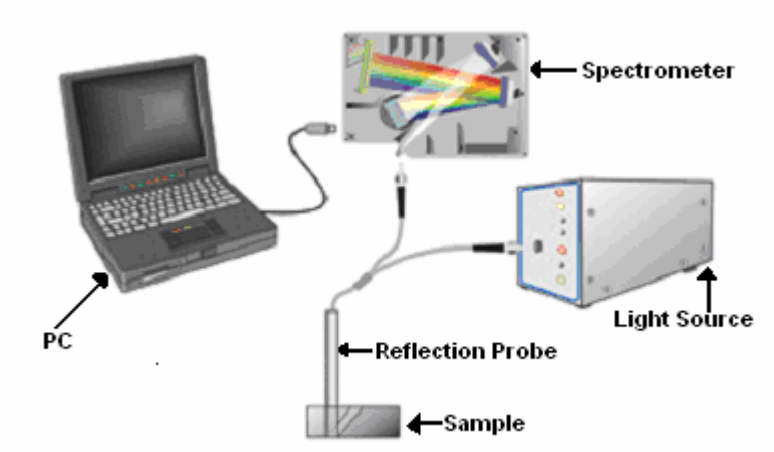
Where:

S_λ = the sample intensity at wavelength λ

D_λ = the dark intensity at wavelength λ

R_λ = the reference intensity at wavelength λ

The following figure shows a typical reflection setup. A light source sends light via the input leg of a reflection probe onto a sample. A reflection probe holder holds the probe in either a 90 or 45-degree angle from the surface. The output leg of the reflection probe carries light from the sample to the spectrometer, which is connected to the computer.



Typical Reflection Setup

Common reflection applications include measuring the properties of mirrors and coatings. Other applications include measuring the visual properties of the color in paints, plastics, and food products.

► *Procedure*

Perform the following steps to take reflection measurements using SpectraSuite:

1. Place SpectraSuite in Scope mode by clicking the Scope ( ) icon in the Experiment mode toolbar or selecting **Processing | Processing Mode | Scope** from the menu.

2. Ensure that the entire signal is on scale.

3. Take a reference spectrum with the WS-1 Diffuse Reflectance Standard or the STAN-SSH High-reflectivity Reference Standard. You must take a reference spectrum before measuring reflection.

4. Click the Store Reference Spectrum ( ) icon on the toolbar or by select **File | Store | Store Reference Spectrum** from the menu bar to store the reference. This command merely stores a reference spectrum in memory. You must click the Save Spectra ( ) icon on the toolbar to permanently save the reference spectrum to disk.

5. Either block the light path to the spectrometer, uncheck the **Strobe/Lamp Enable** box in the Acquisition toolbar, or turn the light source off. Then, take a dark spectrum by clicking the Store Dark Spectrum ( ) icon on the toolbar or by selecting **File | Store | Store Dark Spectrum** from the menu bar. This command merely stores a dark spectrum in memory. You must click the Save Spectra ( ) icon on the toolbar or select **File | Save | Save Spectra Collection** from the menu bar to permanently save the spectrum to disk.

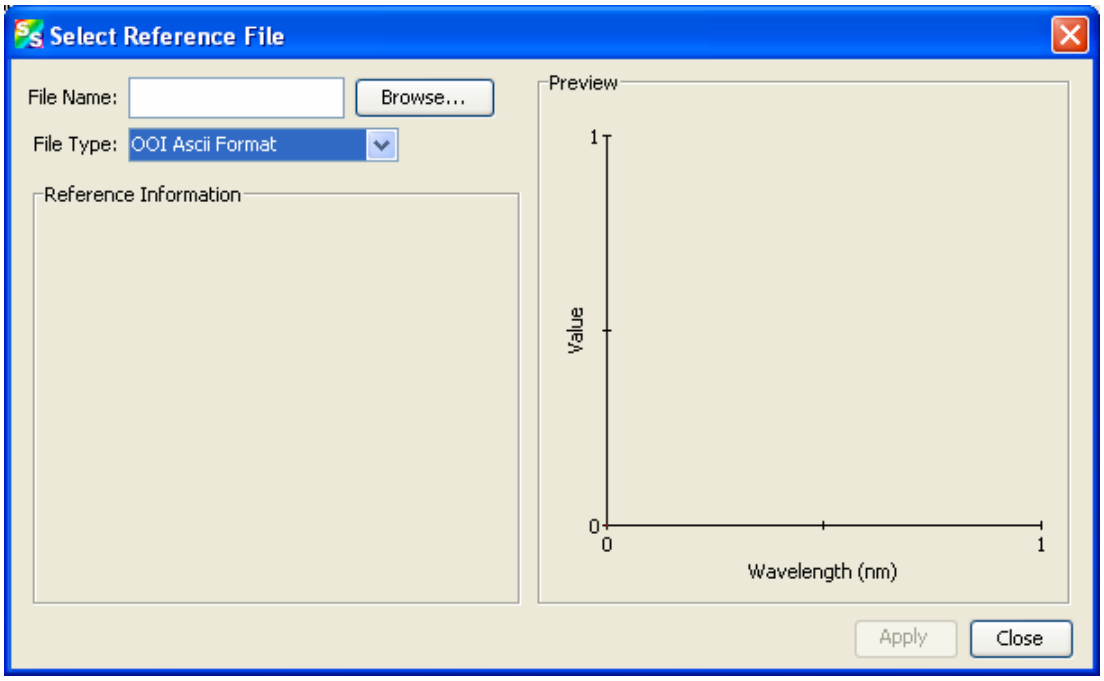
Note

If possible, do not turn off the light source when taking a dark spectrum. If you must turn off your light source to store a dark spectrum, allow enough time for the lamp to warm up again before continuing your experiment.

You must take a dark spectrum before measuring reflection.

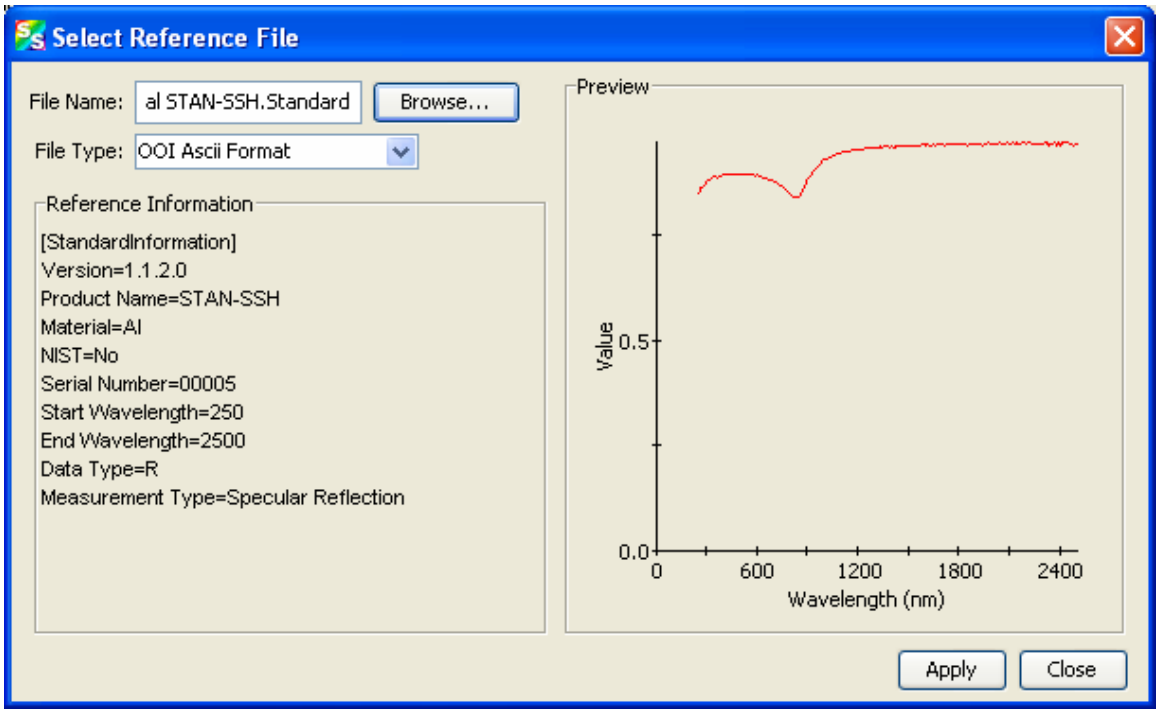
6. Put the sample in place and ensure that the light path is clear. Then, take a reflection measurement by clicking on the Transmission (T) icon on the toolbar or selecting **Processing | Processing Mode | Transmission** from the menu (since the mathematical calculations used to calculate transmission and reflection are identical).

7. If you received calibration file with your reference standard, click the Non-unity Correction icon (≠1) on the toolbar. The **Select Reference File** screen appears.



8. Browse to the location where you stored your reflectivity standard files. Then click the **Apply** button.

   The reference information appears on the **Select Reference File** screen.



9. Click Apply to apply the file data to your graph on the main SpectraSuite screen.

10. To permanently save the spectrum to disk, click the Save Spectra ( ) icon on the toolbar or select **File | Save | Save Spectra Collection** from the menu bar.

Note

If you change any sampling variable (integration time, averaging, smoothing, angle, temperature, fiber size, etc.), you must store a new reference and dark spectrum.

Irradiance Experiments

Irradiance is the amount of energy at each wavelength emitted from a radiant sample. Absolute irradiance is the measure of light in absolute terms. Relative irradiance is a comparison of the fraction of energy the sample emits and the energy the sampling system collects from a lamp with a blackbody energy distribution (normalized to 1 at the energy maximum). SpectraSuite calculates relative irradiance with the following equation:

$$I_\lambda = B_\lambda \left(\frac{S_\lambda - D_\lambda}{R_\lambda - D_\lambda} \right)$$

Where:

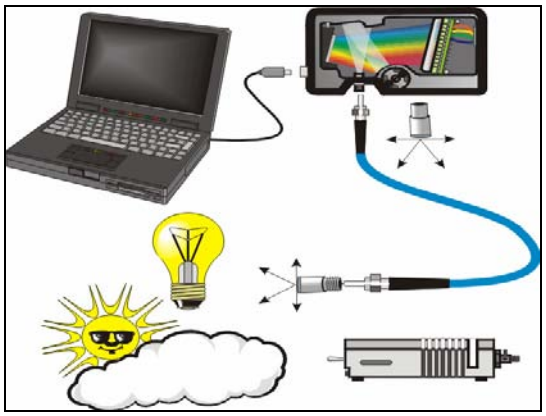
B_λ = Relative energy of the reference (calculated from the color temperature) at wavelength λ

S_λ = Sample intensity at wavelength λ

D_λ = Dark intensity at wavelength λ

R_λ = Reference intensity at wavelength λ

Typical relative irradiance setup: Use a light source with a known color temperature (such as the LS-1 or LS-1-LL (lower right) to take a reference spectrum. The light to measure (lower left) accumulates through a CC-3 Cosine Corrector (or FOIS integrating sphere) into an input fiber, which carries the light information to the spectrometer. The spectrometer then transmits the information to the computer, which compares the measured spectra against the reference spectrum, thus removing wavelength-dependent instrument response from the measurement.



Common applications include characterizing the light output of LEDs, incandescent lamps, and other radiant energy sources such as sunlight. Relative irradiance measurements also include fluorescence measurements, which measure the energy given off by materials excited by light at shorter wavelengths (see *Fluorescence*).

Absolute Irradiance

Although you have the option to do so, you do not need to store reference spectrum first since absolute irradiance is not relative to another measurement. However, you must store a dark spectrum and have a calibration file before you can measure absolute irradiance. Calibration equipment is available from Ocean Optics. Contact an Ocean Optics Application Scientist for more information.

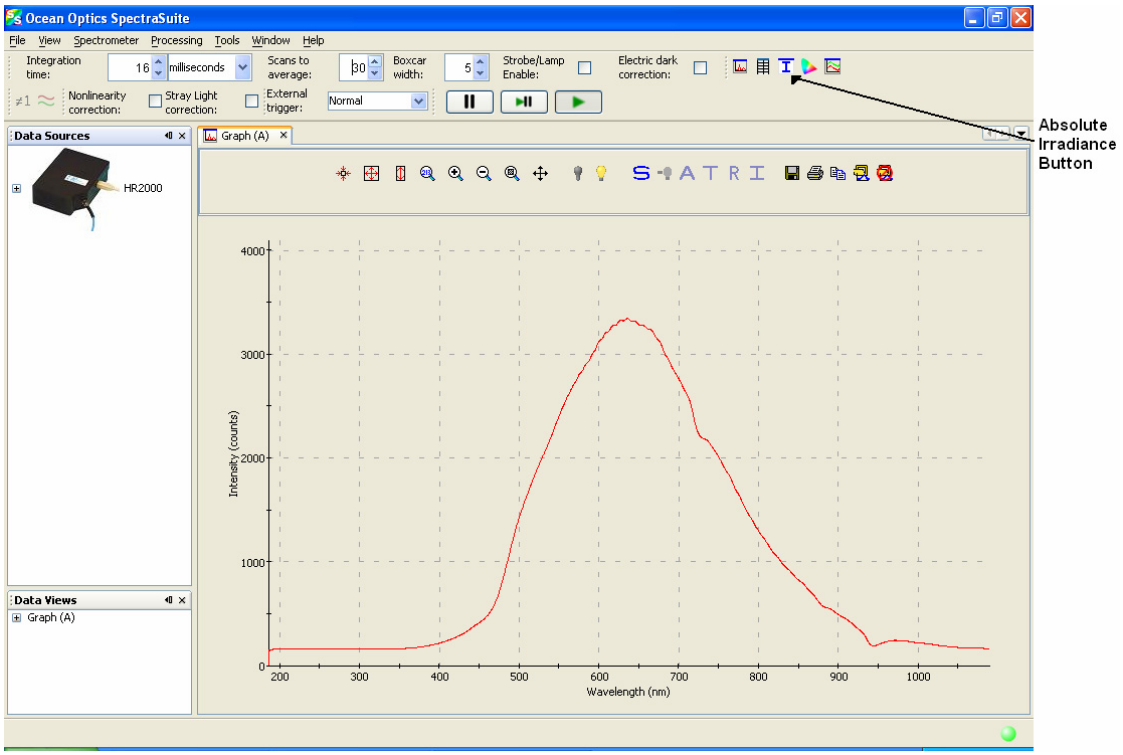
If you select **File | New | Absolute Irradiance Measurement** or click on the Irradiance toolbar, the Absolute Irradiance Wizard is activated to guide you through the process. If you select **File | New | Absolute Irradiance Graph**, the Absolute Irradiance graph in Scope mode appears, and you must work through the various steps required for an Absolute Irradiance measurement on your own.

The following procedure assumes that you are using the Absolute Irradiance Wizard.

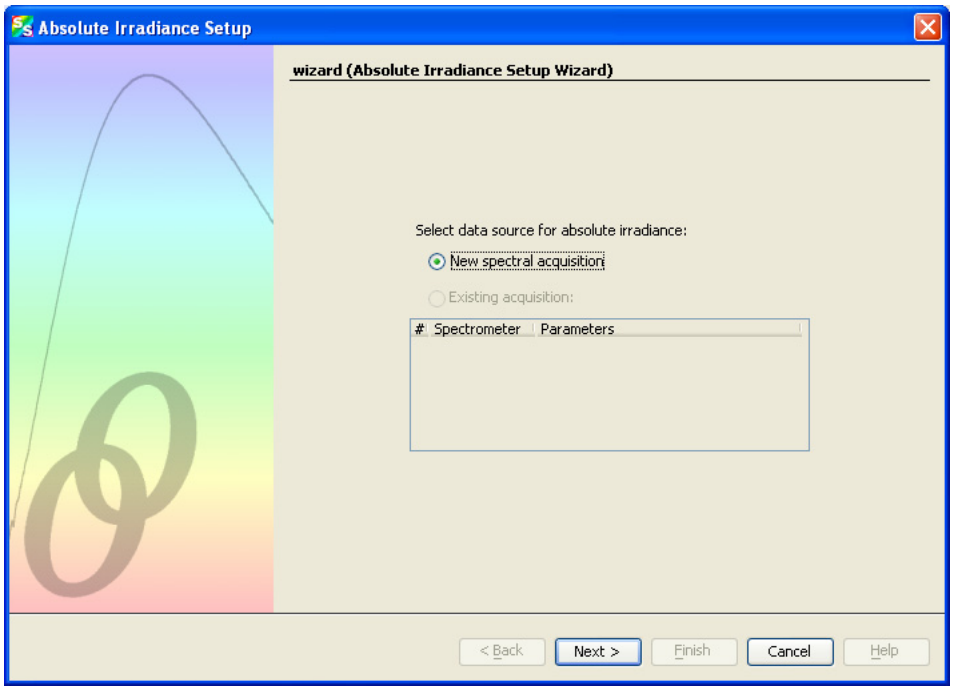
► *Procedure*

Perform the following steps to take an absolute irradiance measurement using SpectraSuite:

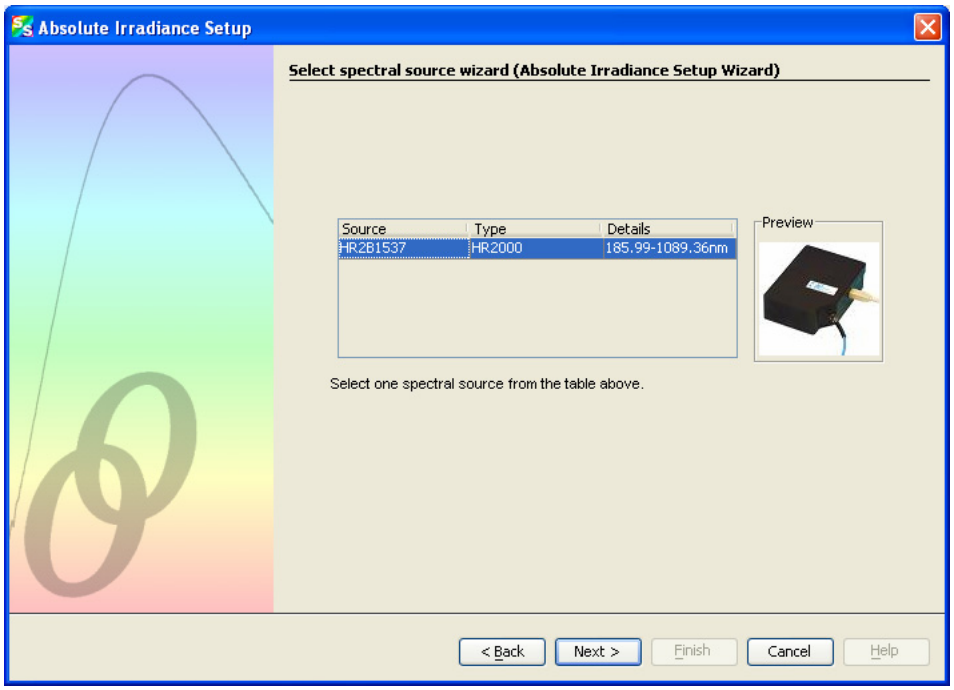
1. Select **File | New | Absolute Irradiance Measurement** from the menu or click on the Irradiance toolbar to use the wizard to create the Absolute Irradiance graph.



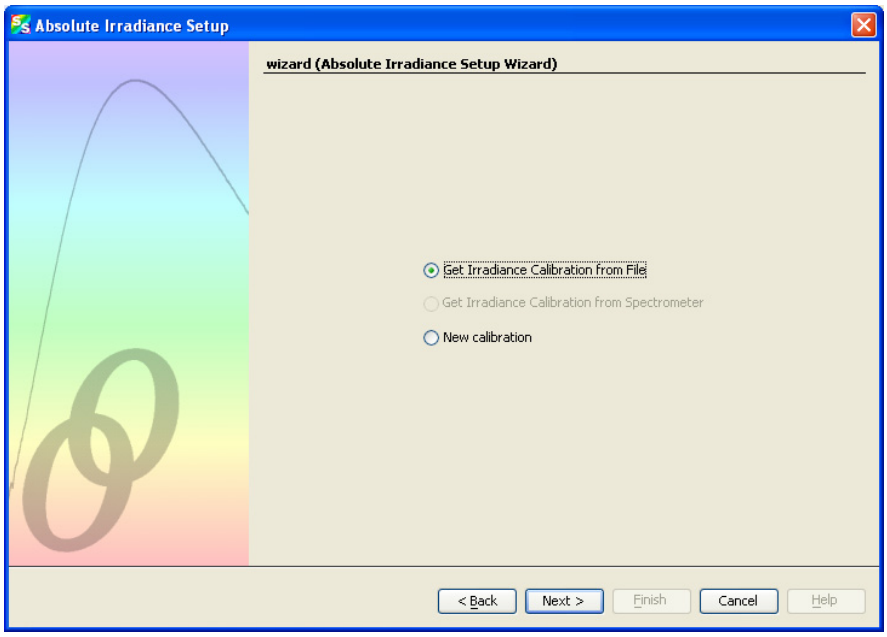
The first page of the Absolute Irradiance Setup Wizard appears.



2. Select to measure absolute irradiance from either a new or existing acquisition. Then, click Next >. The second page of the Absolute Irradiance Setup Wizard appears.



3. If you have more than one spectrometer, highlight the one to be used. Then, click Next >. The third page of the Absolute Irradiance Setup Wizard appears.

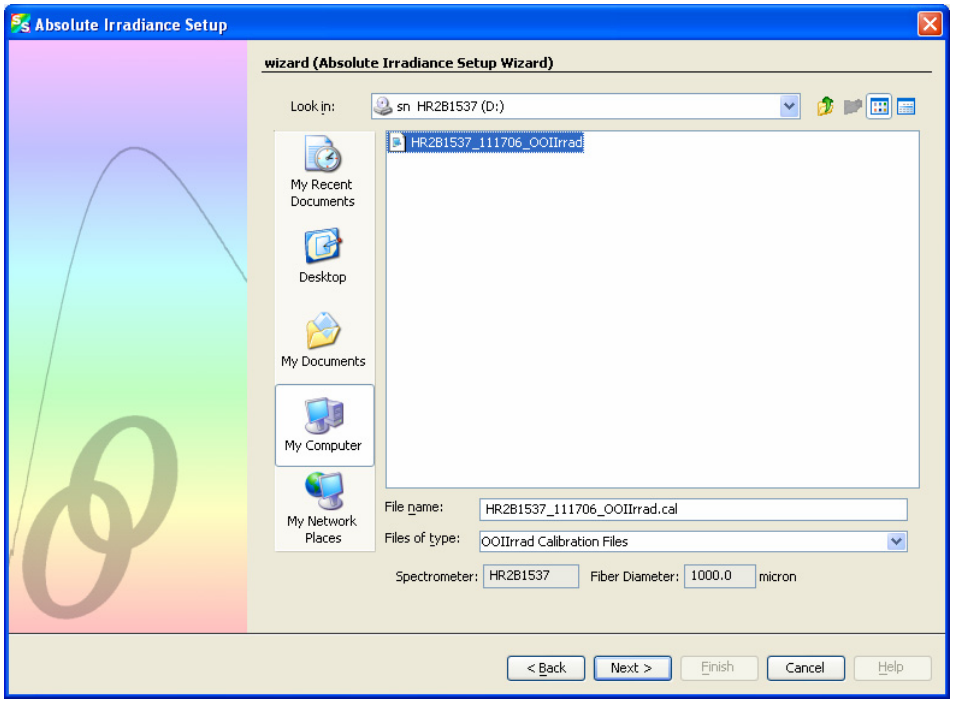


8. Choose one of the following:

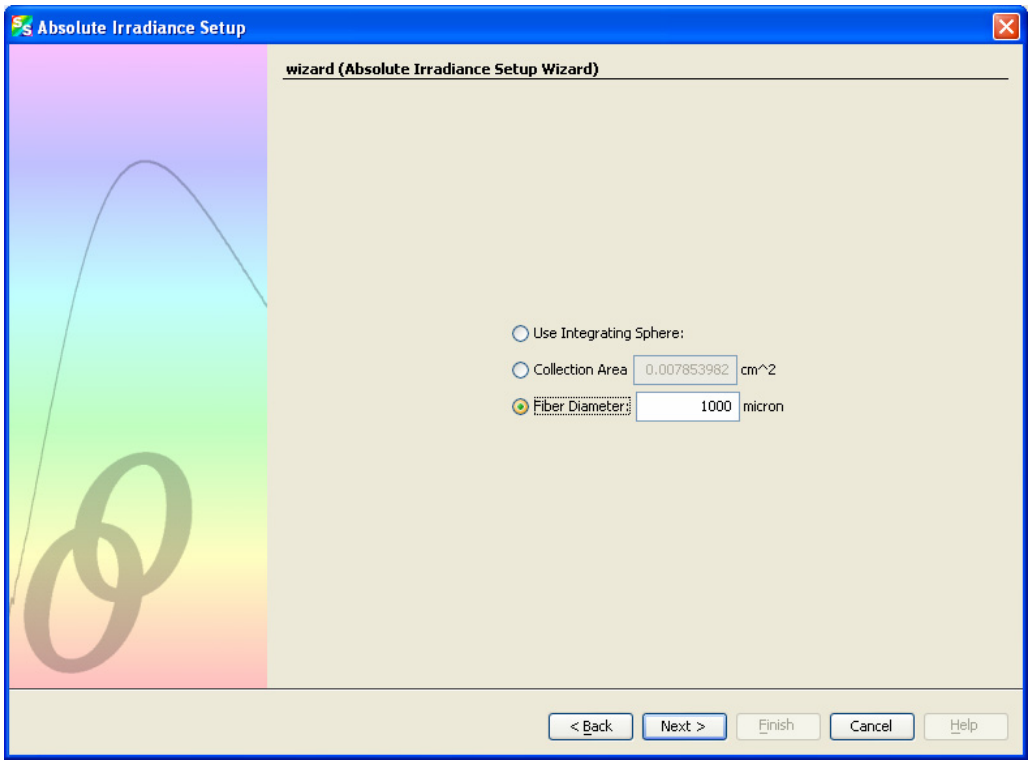
   - ***Get Irradiance Calibration from File***
   - ***New Calibration***

Get Irradiance Calibration from File

a. After selecting **Get Irradiance Calibration from File**, browse to the desired calibration file.



b. Select the file and click Next >.



c. If you are using an integrating sphere, check the **Use Integrating Sphere** option.

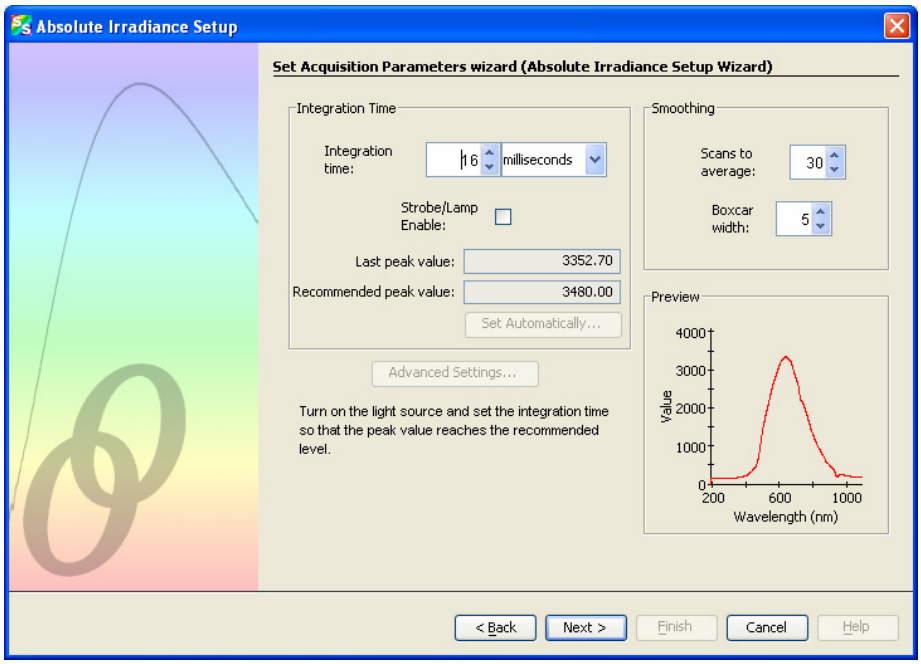
d. If you know the collection area, check Collection Area and enter the value.

e. If you are using a bare fiber or a cosine corrector, check **Fiber Diameter** and enter the value.

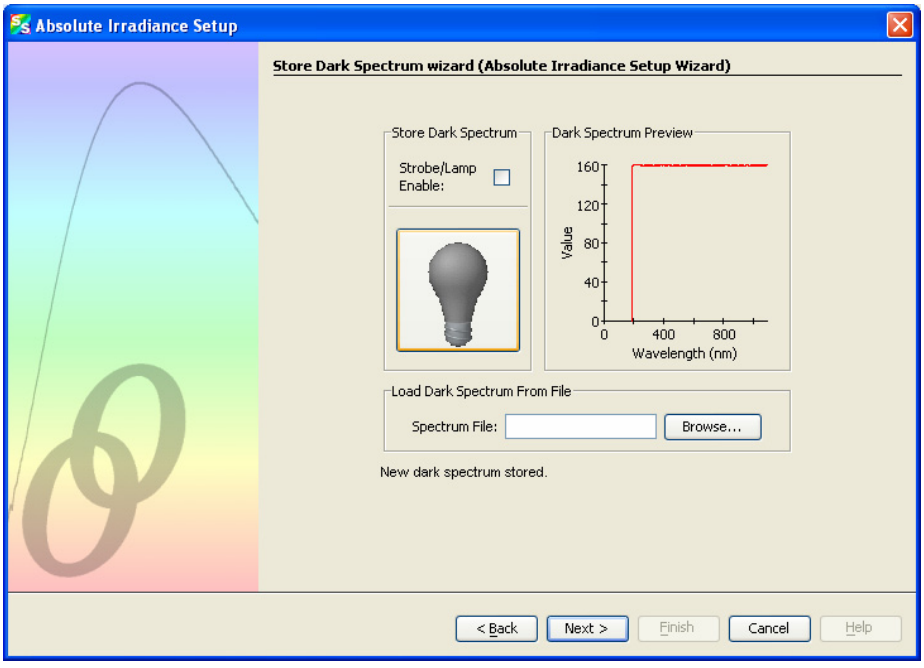
f. If you are using an Ocean Optics cosine corrector or a direct attach cosine corrector, enter the appropriate value for the Fiber Diameter as follows:

Cosine Corrector	Fiber Diameter
CC-3	3900 microns
CC-3-UV	3900 microns
CC-3-DA	7140 microns

g. Then click Next >. The **Set Acquisition Parameters** screen appears.



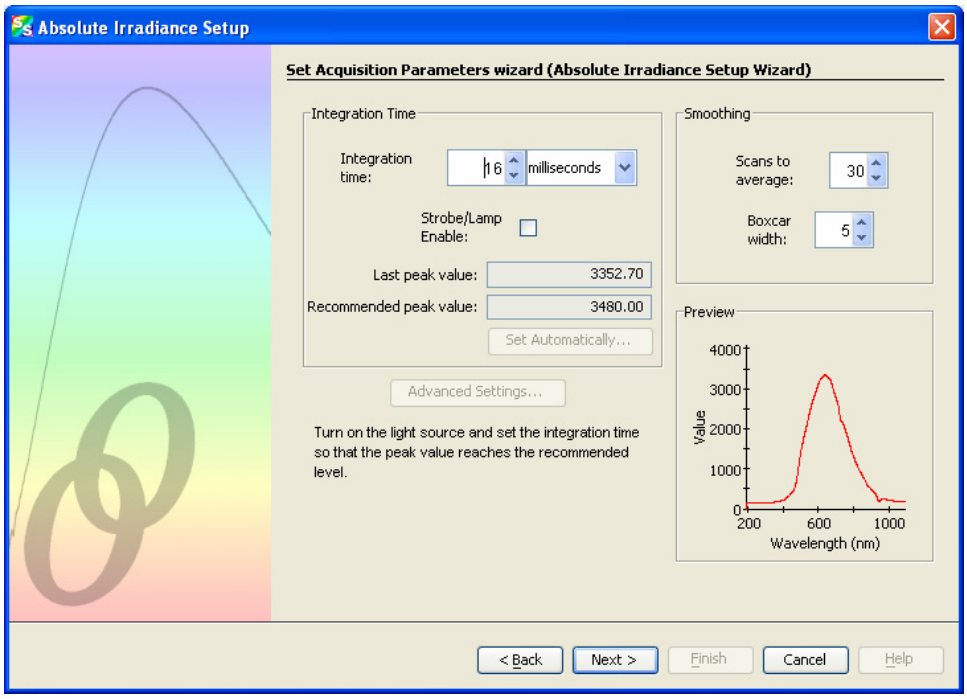
h. Set your acquisition parameters for your experiment using the **Integration time** and **Boxcar width** so that the **Last peak value** is very close to the **Recommended peak value**. Then, click Next >. The Dark Spectrum screen appears.



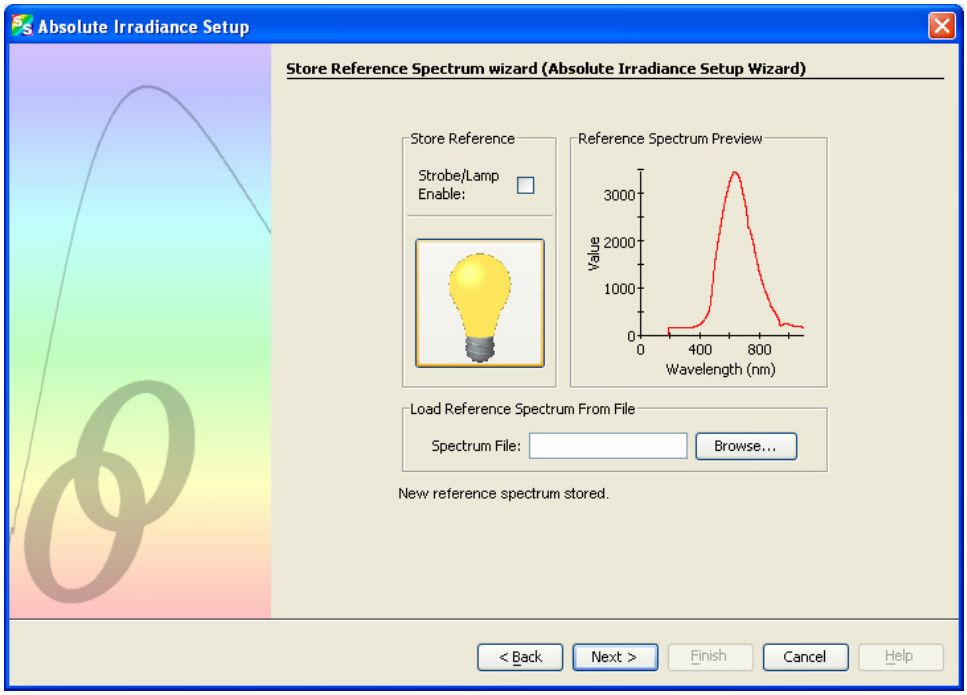
i. Block the light path or uncheck the **Strobe/Lamp Enable** box, then click to take a dark spectrum. The graph appears on the right side of the screen. Click Finish.

New Calibration

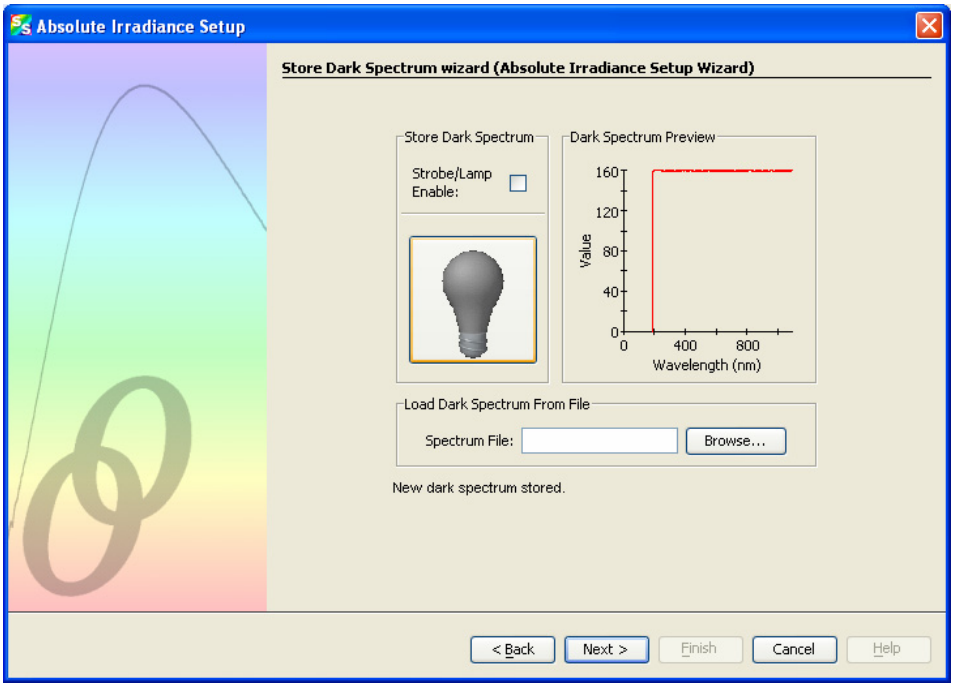
a. After selecting New Calibration, the Set Acquisition Parameters screen appears.

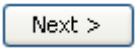


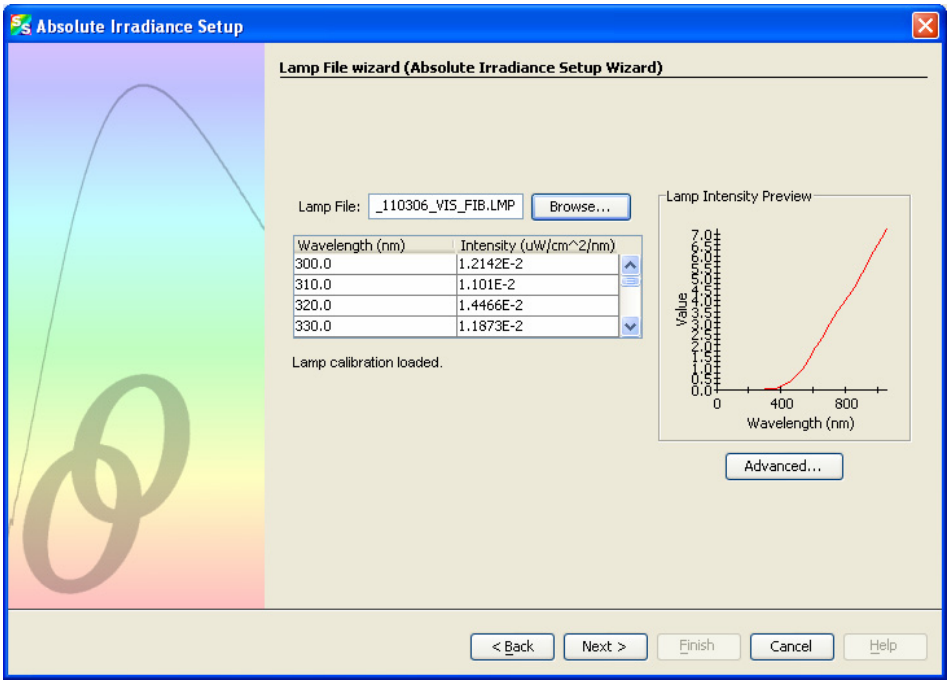
b. Set your acquisition parameters for your experiment. Then, click Next >. The Store Reference screen appears.



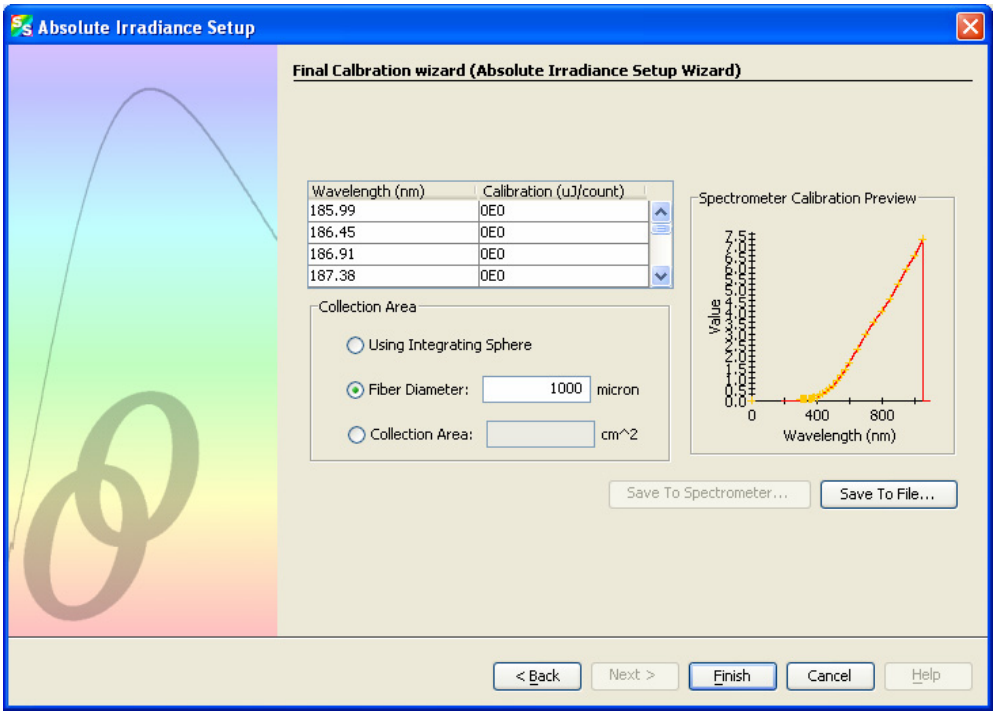
c. Turn on your light source, then click to store a reference spectrum. The Dark Spectrum screen appears.



d. Block the light path or uncheck the Strobe/Lamp Enable box, then click to take a dark spectrum. The graph appears on the right side of the screen. Click  . The Lamp File wizard screen appears.



e. Enter the name of the lamp file or browse to the desired file to use. The final screen of the calibration wizard appears. Note in the **Spectrometer Calibration Preview** that the lamp file curve (in yellow) is overlayed on the spectrometer's curve (red). Once you apply this calibration, the curves should be exactly the same.



f. Click Finish. The **Absolute Irradiance Calibration** measurement screen appears.

Relative Irradiance

Relative irradiance is a measurement of light relative to the known color temperature of a blackbody light source. Common applications include characterizing the light output of LEDs, incandescent lamps, and other radiant energy sources such as sunlight. Relative irradiance measurements also include fluorescence measurements, which measure the energy given off by materials excited by light at shorter wavelengths. You must have stored reference and dark spectra before measuring relative irradiance.

► *Procedure*

1. Place SpectraSuite in Scope mode by clicking the Scope ( ) icon in the Experiment mode toolbar or selecting **Processing | Processing Mode | Scope** from the menu.

2. Ensure that the entire signal is on scale. The intensity of the reference signal's peak differs depending on the device being used. If necessary, adjust the integration time until the intensity is appropriate for your device.

3. Take a reference spectrum using a light source with a black body of a known color temperature, such as the LS-1.

4. Click the Store Reference Spectrum ( ) icon on the toolbar or by select **File | Store | Store Reference Spectrum** from the menu bar to store the reference. This command merely stores a reference spectrum in memory. You must click the Save Spectra ( ) icon on the toolbar or select **File | Save | Save Spectra Collection** from the menu bar to permanently save the reference spectrum to disk.

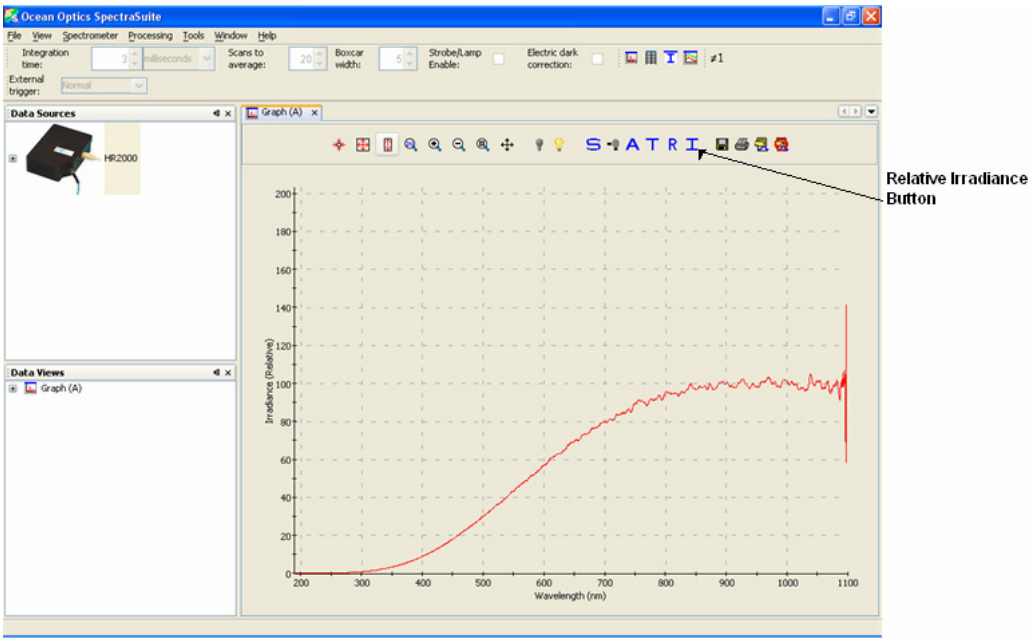
5. If you have not already done so, store a dark spectrum reading. To do this, either block the light path to the spectrometer, uncheck the **Strobe/Lamp Enable** box in the Acquisition toolbar, or turn the light source off. Then, take a dark spectrum by clicking the Store Dark Spectrum ( ) icon on the toolbar or by selecting **File | Store | Store Dark Spectrum** from the menu bar. This command merely stores a dark spectrum in memory. You must click the Save Spectra ( ) icon on the toolbar.

Note

If possible, do not turn off the light source when taking a dark spectrum. If you must turn off your light source to store a dark spectrum, allow enough time for the lamp to warm up again before continuing your experiment.

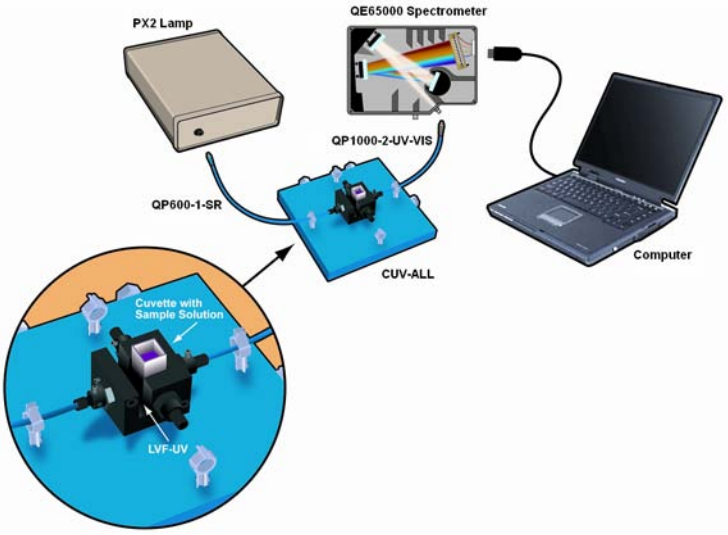
You must take a dark spectrum before measuring relative irradiance.

6. Position the fiber at the light source you want to measure. Then, click . The Relative Irradiance graph appears.



Fluorescence

A fluorescence measurement is a type of relative irradiance measurement in which the energy given off by materials excited by light at shorter wavelengths is measured. Advantages of fluorescence include High sensitivity, high speed (intensity changes on the order of picoseconds), and safety (nondestructive to sample and no hazardous by-products). A typical fluorescence set-up is shown below. Note that the fibers for the lamp and the spectrometer must be at a 90° angle to each other (or a CVD-DIFFUSE must be used).

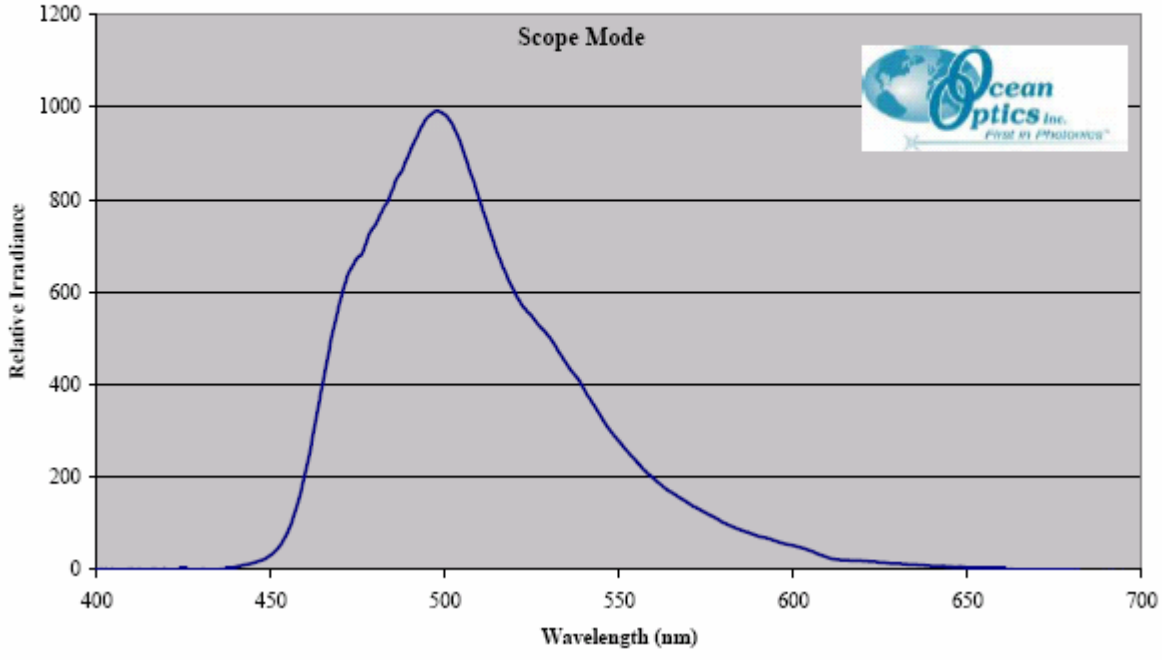


Fluorescence can be measured in the following modes:

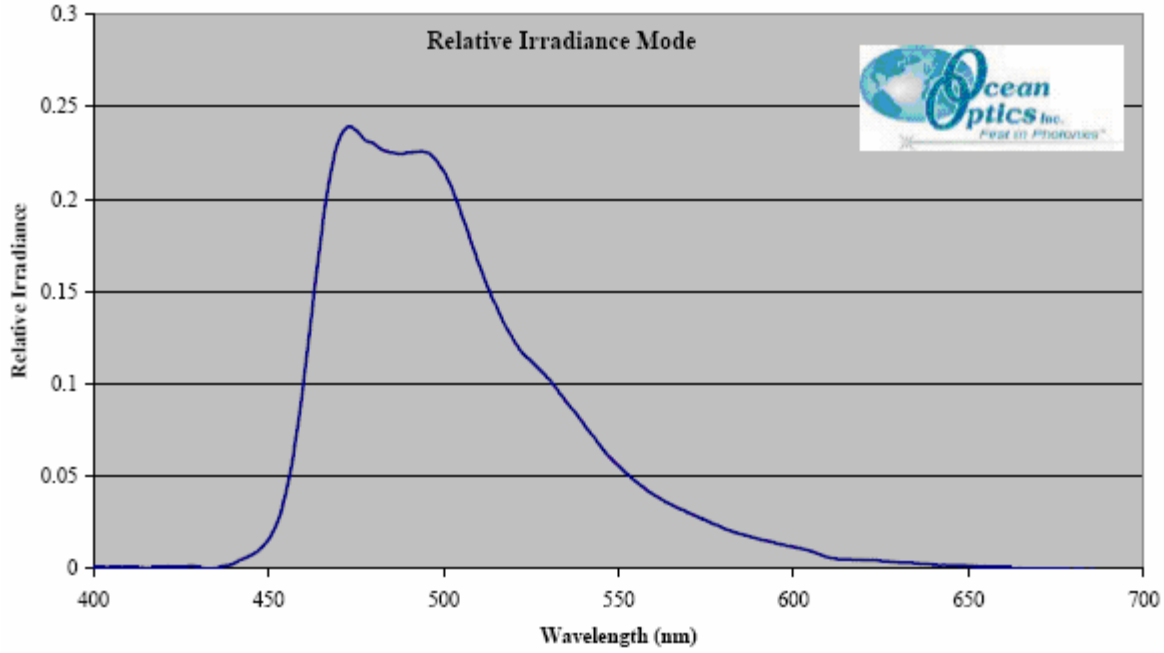
- Scope mode: Scope mode is the preferred mode for configuring your acquisition parameters. The signal graphed in Scope mode is the raw voltage coming out of the A/D converter. This spectral view mode provides complete control of signal processing functions before taking absorbance, transmission, reflection, and relative irradiance measurements. This mode reflects the intensity of the light source, the reflectivity of the grating and mirrors in the spectrometer, the response of the detector, and the spectral characteristics of the sample.
- Relative Irradiance mode: Relative Irradiance mode is the preferred mode for fluorescence experiments. Relative irradiance spectra are a measure of the intensity of a light source relative to a reference emission source. There are two methods of performing a fluorescence experiment in Relative Irradiance mode: run SpectraSuite in Relative Irradiance mode using the calibration files generated during factory calibration, or perform your own radiometric calibration using a blackbody of known color temperature. See *Relative Irradiance* for the experiment procedure.

See the following figures for examples of graphs of relative irradiance in a fluorescence measurement.

PVK sample measured with the USB2000-FL spectrometer, PX2 pulsed xenon light source, CUV-ALL-4-Way cuvette holder, 1000 um illumination fiber, 600 um detection fiber
Sample in disposable cuvette



PVK sample measured with the USB2000-FL spectrometer, PX2 pulsed xenon light source, CUV-ALL-4-Way cuvette holder, 1000 um illumination fiber, 600 um detection fiber (LS-1 tungsten halogen light source used for reference) Sample in disposable cuvette



Note

If you have a spectrometer with a gated detector (such as the USB2000-FLG), you can initiate a fluorescence measurement with **File | New | New Gated Fluorescence Measurement**.

If you have a Curie UV-VIS Emission Spectrofluorometer (serial number starts with CUR), you can initiate a fluorescence measurement with **File | New | New Curie Fluorescence Measurement**.

Application Tips

If the signal you collect . . .	You can . . .	By . . .
Saturates the spectrometer (peaks are off the scale)	Decrease the light level on scale in Scope mode	• Decreasing the integration time, or • Incorporating linear variable filters into your experiment
Has too little light	Increase the light level on scale in Scope mode	• Increasing the integration time, or • Removing linear variable filters from the light path

Color Experiments

With SpectraSuite, you can obtain photopic data (in either lumens or lux per unit area) based on a CIE standard visibility curve. You can also control the parameters for all system and display functions, such as data acquisition, graph display, and cursor configuration. In addition, you can create a spreadsheet display of lamp output intensity by wavelength, providing an easy way to chart and analyze acquired data. SpectraSuite will compute all color measurements except RGB.

► *Procedure*

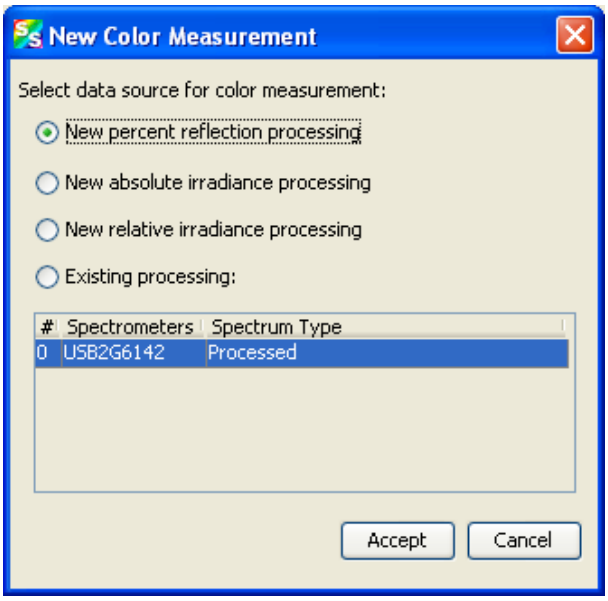
To collect color data,

1. From the main graph, click the Chromaticity icon on the Processing toolbar

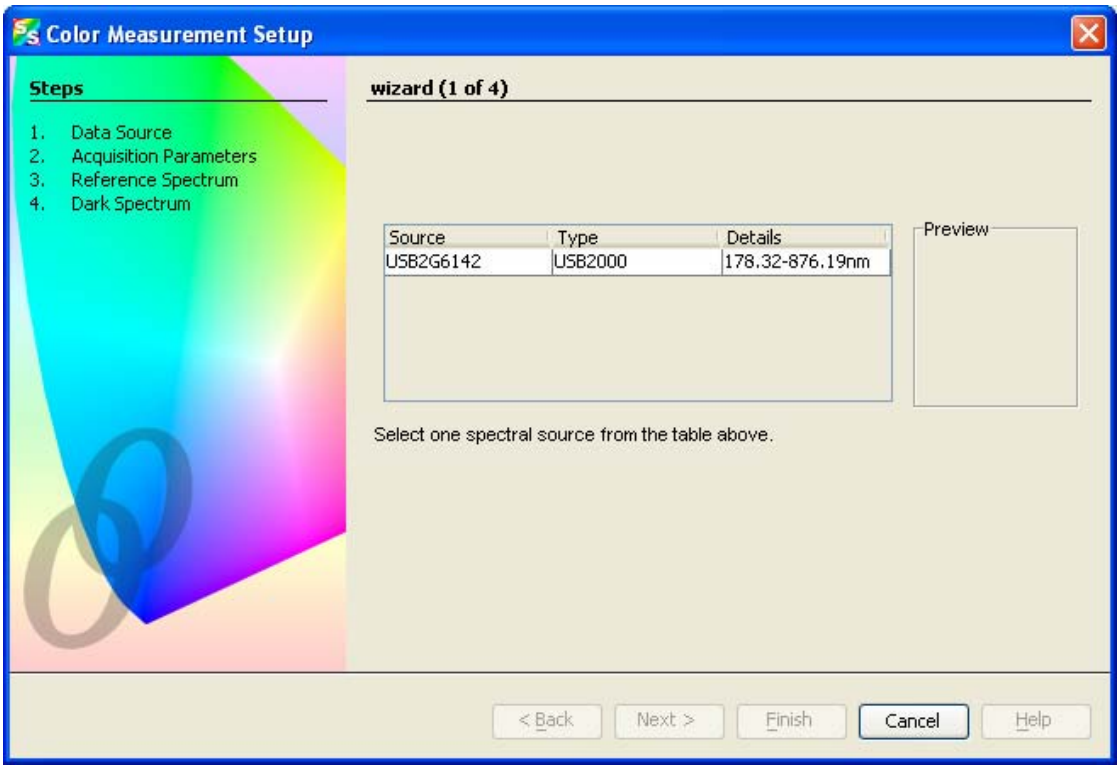
   OR

   Select **File | New | Color Measurement**.

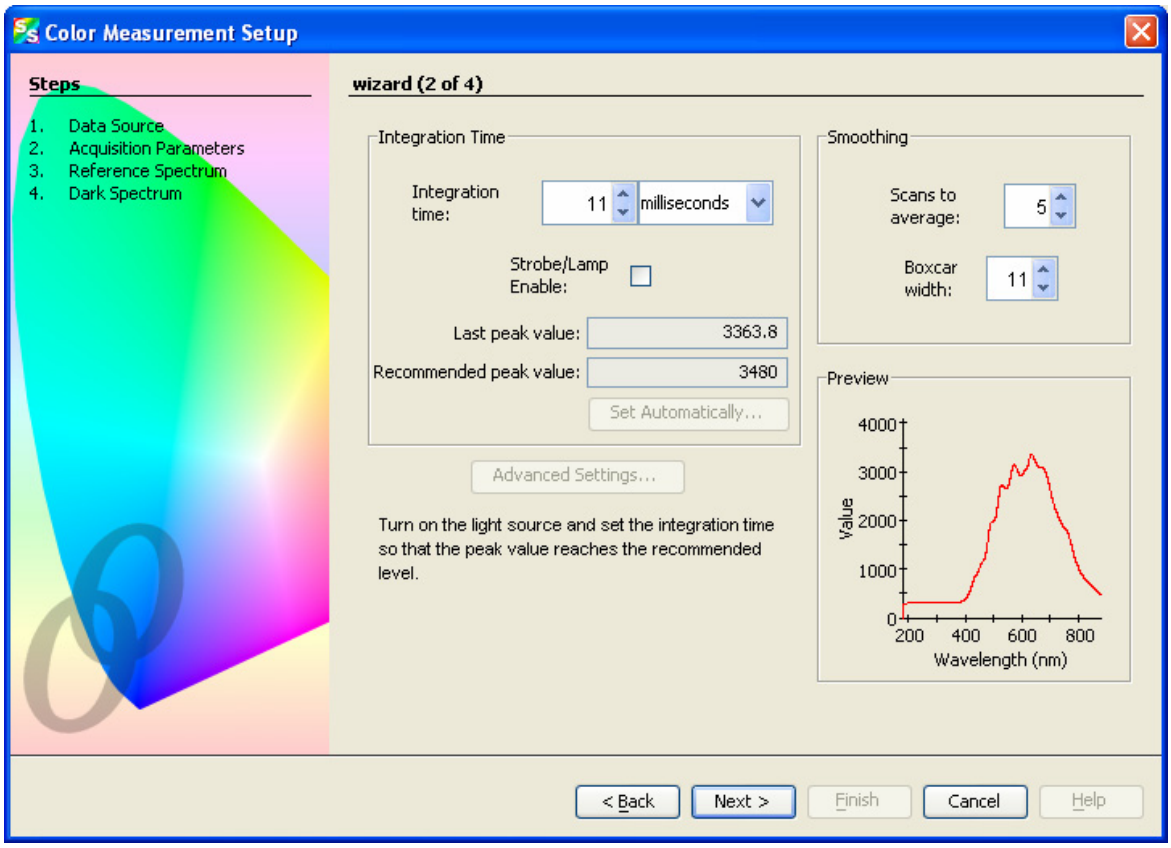
   The **New Color Measurement** dialog box appears.



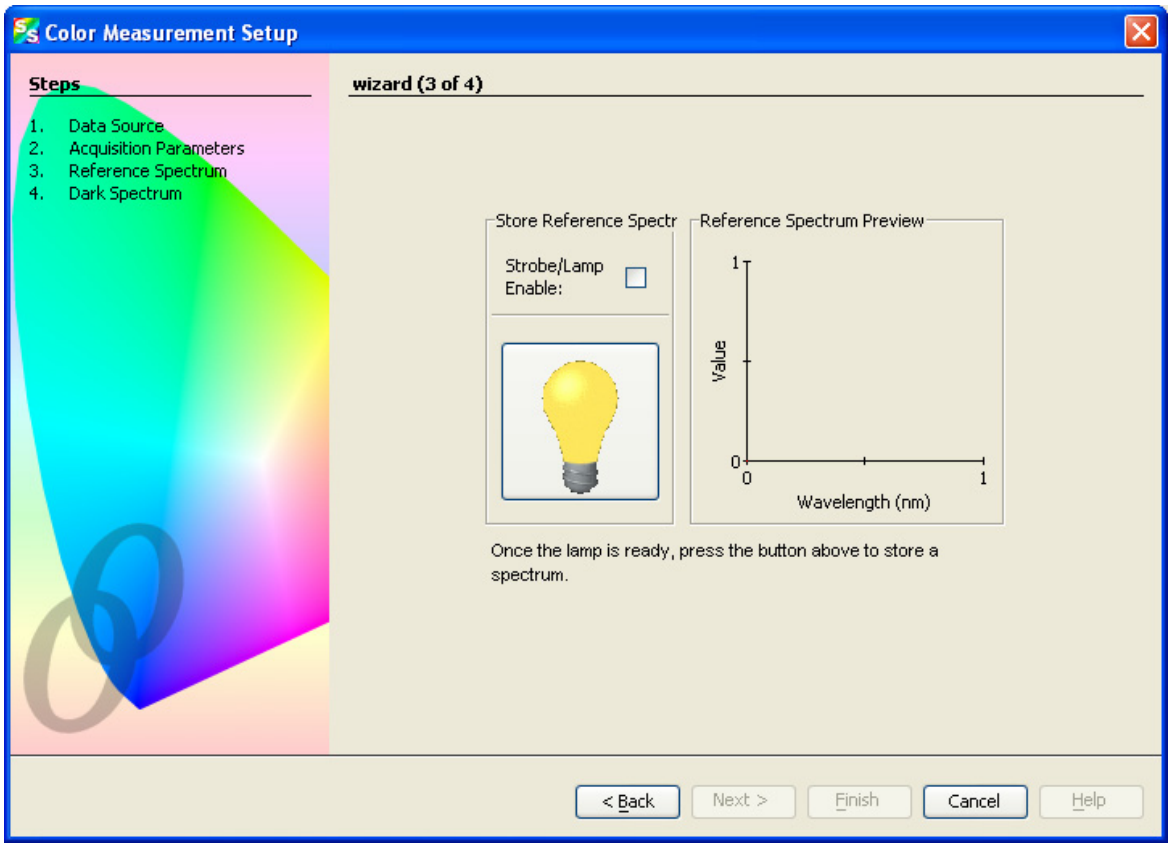
2. Select the data source for the color measurement and click Accept. The first Color Measurement Setup wizard screen appears.



3. Highlight the desired spectral source to select it. Then click Next >. The second Color Measurement Setup wizard screen appears.

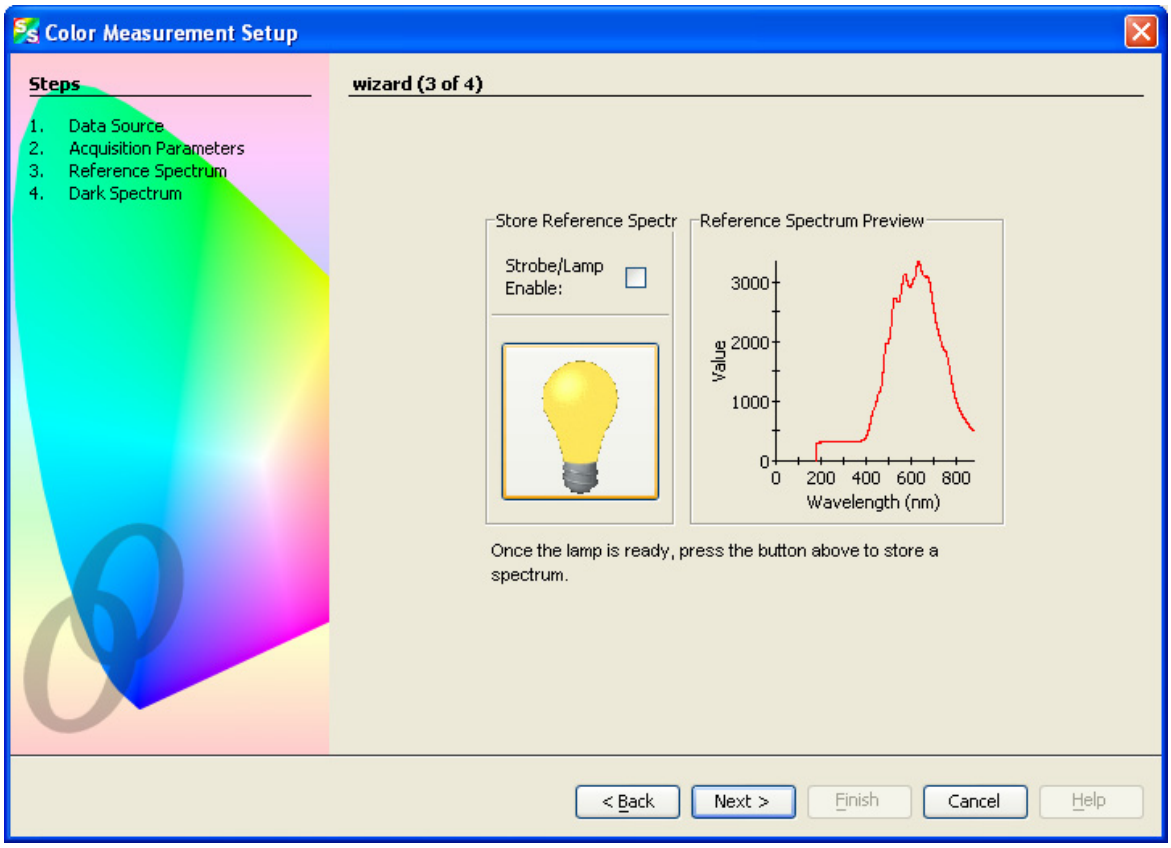


4. Turn on your light source. Adjust the **Integration time**, **Scans to average**, and **Boxcar width** so that the **Last peak value** is within the proper range (near the **Recommended peak value**). When this happens, the **Last peak value** reading changes from pink to black. Then, click Next >. The third Color Measurement Setup wizard screen appears.

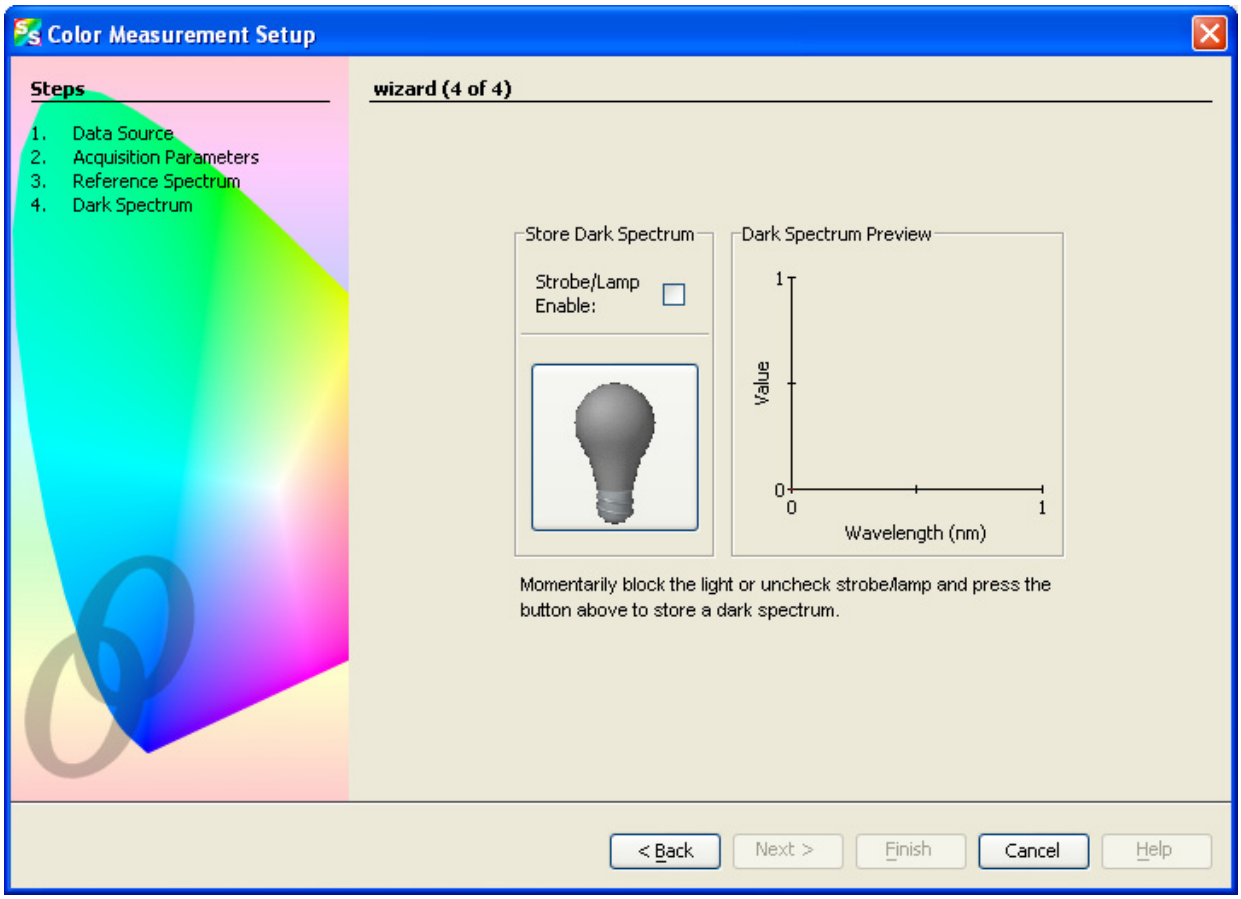


If you are performing an absolute irradiance calibration, go on to Step 6. Otherwise, continue with Step 5.

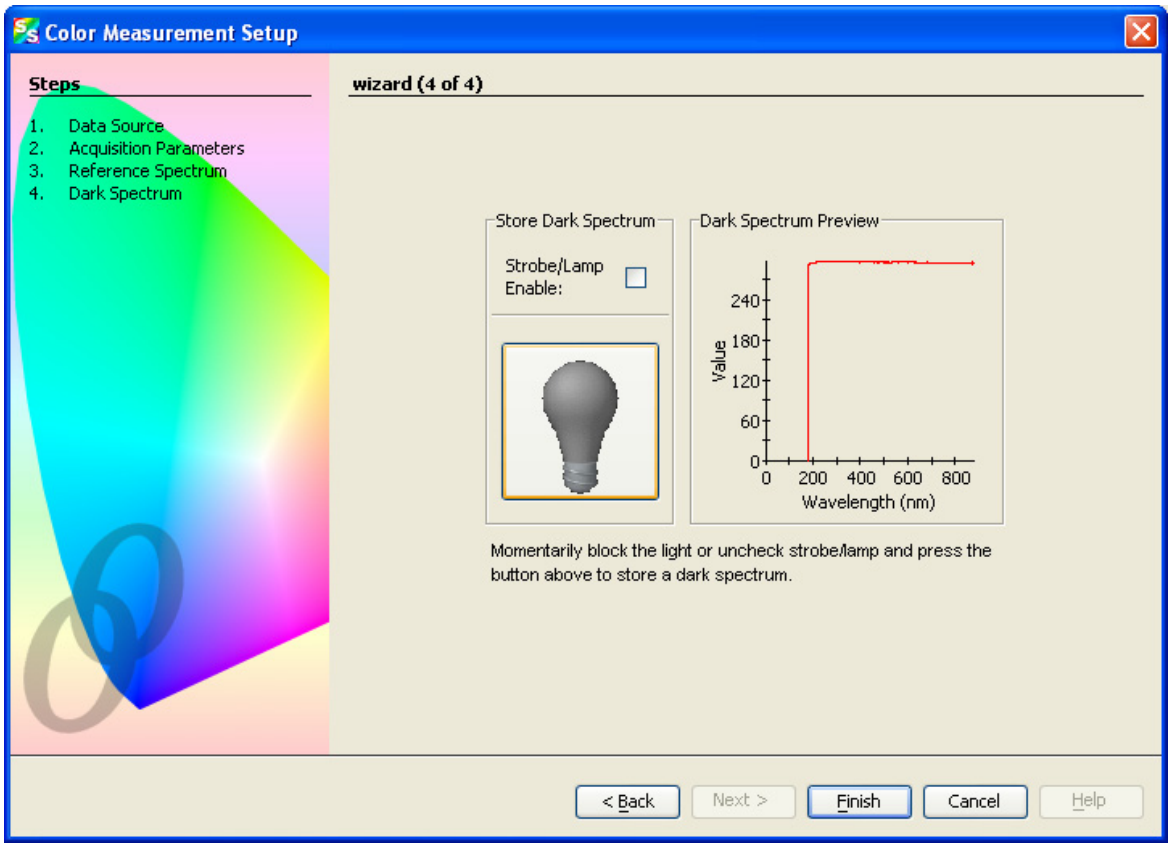
5. If you have not done so already, check the **Strobe/Lamp Enable** box or physically turn on the lamp. Once the lamp has warmed up, click to store a reference spectrum. The graph appears in **Reference Spectrum Preview**.



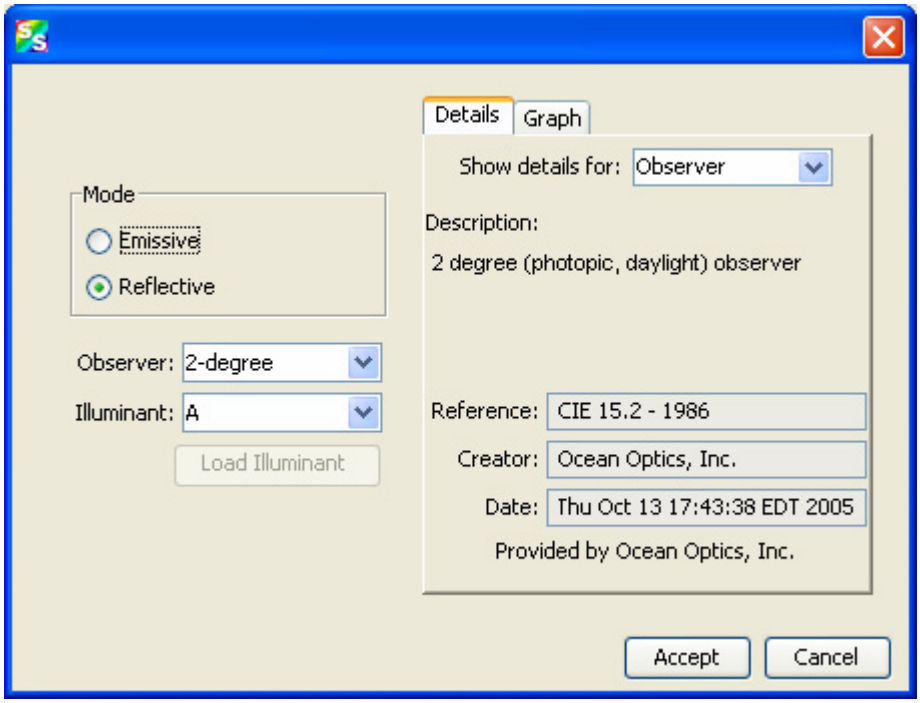
6. Click Next >. The fourth Color Measurement Setup wizard screen appears.



7. Block the light or uncheck **Strobe/Lamp Enable**. Then click to store a dark reference spectrum. The graph appears in **Dark Spectrum Preview**.



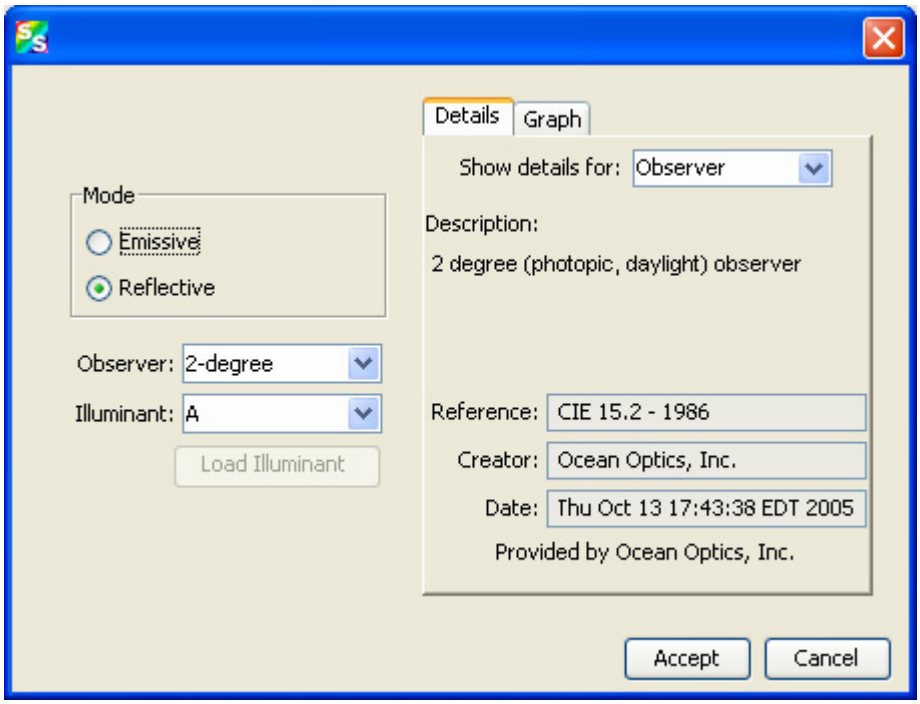
8. Click Finish. The following screen appears.



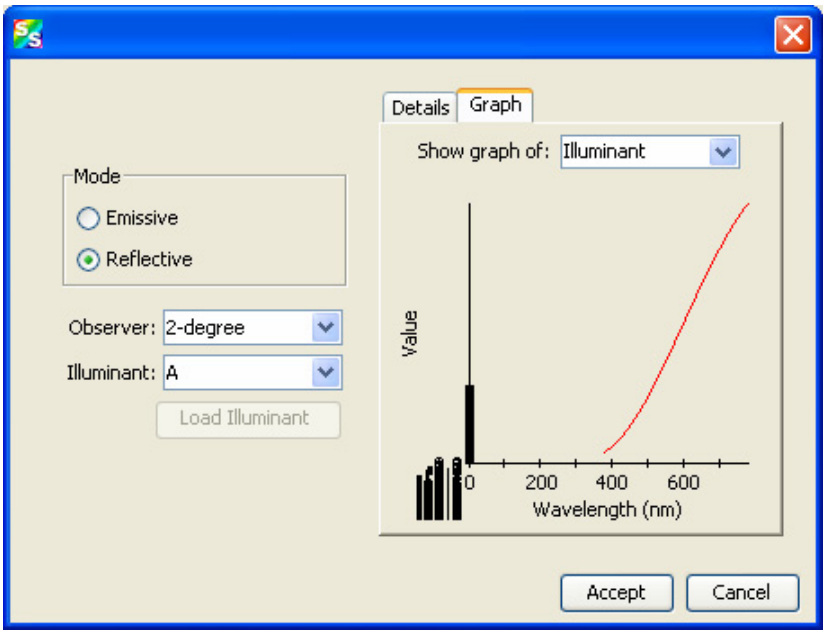
The fields on this screen are described in the following table.

Field	Description
Mode	Either Emissive or Reflective mode is selected, depending on the type of color measurement selected in Step 1. You can change it here: **Reflective** – Color measurement of a surface for a selectable CIE-defined illuminant. **Emissive** - Measurement of the light emitted from an LED or a lamp (emission source).
Observer	Specify the observer (viewing angle) using the drop-down list: **2° (CIE 1931) –** photopic (daylight) **10° (CIE 1964) –** scotopic (dark-adjusted)
Illuminant	If you chose Reflective measurement under **Mode**, select the desired Illuminant from the drop-down list. This illuminant is theoretical and CIE-defined; it has nothing to do with the actual lamp used in the measurement.
Load Illuminant	For future use.

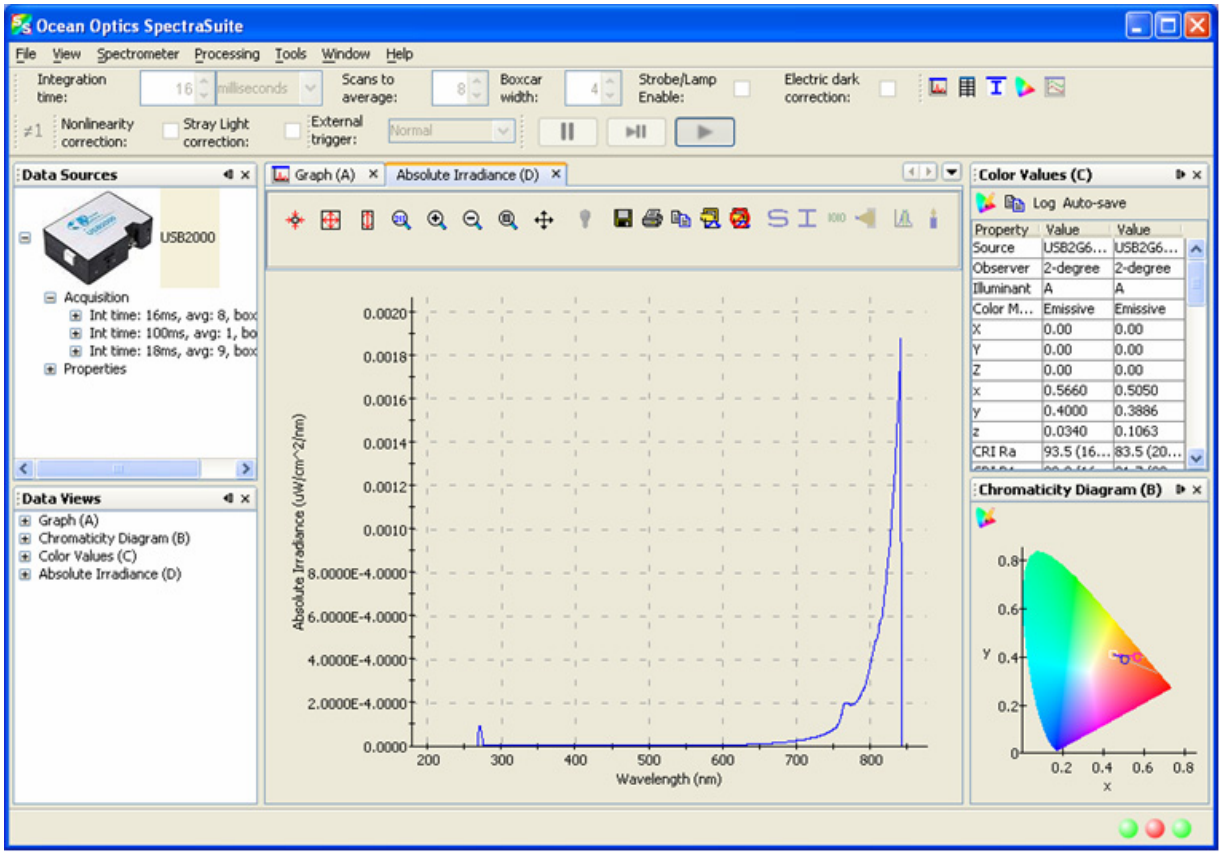
9. Your selections are reflected on the right side of the screen. Select to view either illuminant or observer details in the **Show details for** field. An example screen with details for the observer is shown below:



10. Select the Graph tab to view a graph reflecting the selections you have chosen. An example graph of the illuminant is shown below:



11. Click Accept. Your color data appears on the main SpectraSuite screen as shown below:



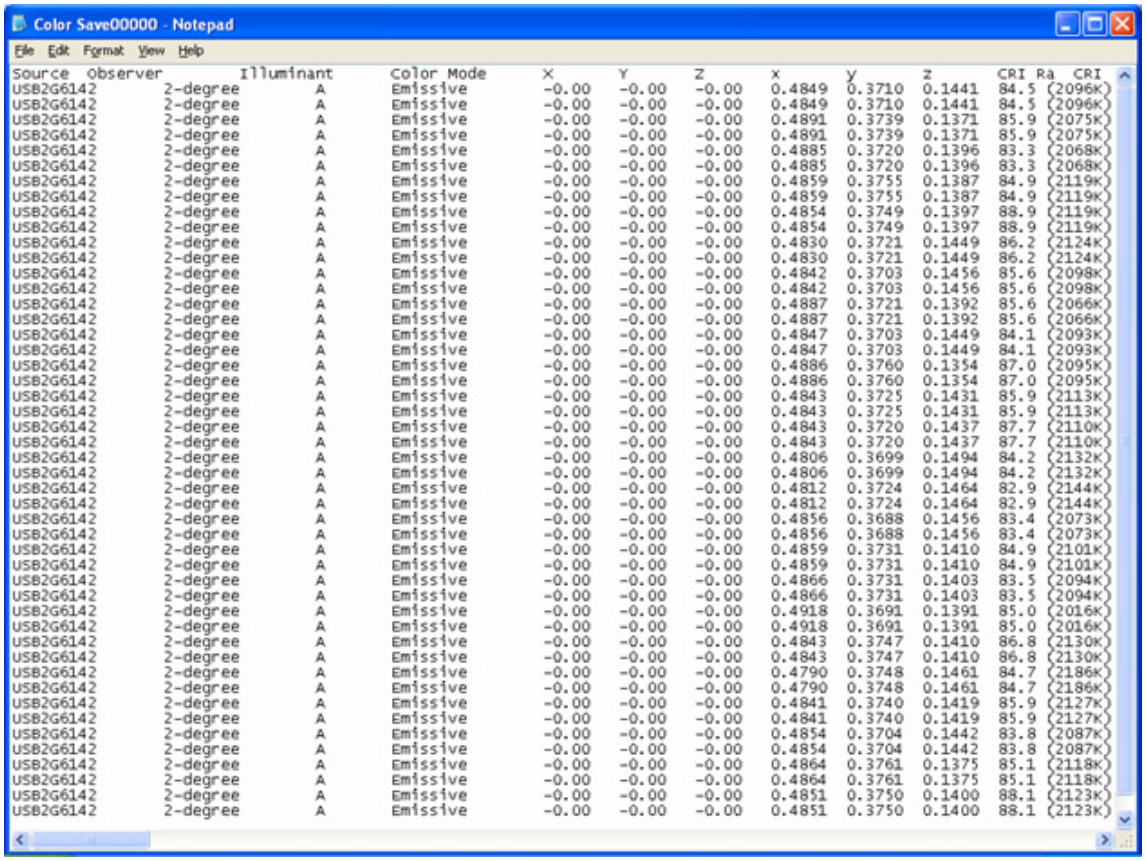
Tip

To close all three color views (**Graph**, **Color Values**, and **Chromaticity Diagram**) at once, highlight the color acquisition in the **Data Sources** pane, right-click and select **Terminate**.

Color Measurement Screen Controls

Once you have captured your color data on the Color Measurement screen shown above, you can use the following controls in the Color Values section of the screen:

Control	Action
	Edit Color settings. Use this control to edit the color settings in your graph. See *Edit Color Settings* for more information.
	Copy Spectral Data to Clipboard.
Log	Opens a browser for you to select a log file you have created.
Auto-save	Saves your color data to a file. See below for an example saved in Notepad. See *Exporting Processed Data* for more information



Color Save00000 - Notepad

File Edit Format View Help

Source	Observer	Illuminant	Color Mode	X	Y	Z	x	y	z	CRI Ra	CRI
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4849	0.3710	0.1441	84.5	(2096K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4849	0.3710	0.1441	84.5	(2096K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4891	0.3739	0.1371	85.9	(2075K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4891	0.3739	0.1371	85.9	(2075K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4885	0.3720	0.1396	83.3	(2068K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4885	0.3720	0.1396	83.3	(2068K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4859	0.3755	0.1387	84.9	(2119K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4859	0.3755	0.1387	84.9	(2119K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4854	0.3749	0.1397	88.9	(2119K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4854	0.3749	0.1397	88.9	(2119K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4830	0.3721	0.1449	86.2	(2124K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4830	0.3721	0.1449	86.2	(2124K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4842	0.3703	0.1456	85.6	(2098K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4842	0.3703	0.1456	85.6	(2098K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4887	0.3721	0.1392	85.6	(2066K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4887	0.3721	0.1392	85.6	(2066K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4847	0.3703	0.1449	84.1	(2093K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4847	0.3703	0.1449	84.1	(2093K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4886	0.3760	0.1354	87.0	(2095K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4886	0.3760	0.1354	87.0	(2095K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4843	0.3725	0.1431	85.9	(2113K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4843	0.3725	0.1431	85.9	(2113K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4843	0.3720	0.1437	87.7	(2110K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4843	0.3720	0.1437	87.7	(2110K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4806	0.3699	0.1494	84.2	(2132K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4806	0.3699	0.1494	84.2	(2132K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4812	0.3724	0.1464	82.9	(2144K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4812	0.3724	0.1464	82.9	(2144K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4856	0.3688	0.1456	83.4	(2073K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4856	0.3688	0.1456	83.4	(2073K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4859	0.3731	0.1410	84.9	(2101K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4859	0.3731	0.1410	84.9	(2101K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4866	0.3731	0.1403	83.5	(2094K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4866	0.3731	0.1403	83.5	(2094K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4918	0.3691	0.1391	85.0	(2016K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4918	0.3691	0.1391	85.0	(2016K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4843	0.3747	0.1410	86.8	(2130K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4843	0.3747	0.1410	86.8	(2130K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4790	0.3748	0.1461	84.7	(2186K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4790	0.3748	0.1461	84.7	(2186K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4841	0.3740	0.1419	85.9	(2127K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4841	0.3740	0.1419	85.9	(2127K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4854	0.3704	0.1442	83.8	(2087K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4854	0.3704	0.1442	83.8	(2087K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4864	0.3761	0.1375	85.1	(2118K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4864	0.3761	0.1375	85.1	(2118K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4851	0.3750	0.1400	88.1	(2123K)
USB2G6142	2-degree	A	Emissive	-0.00	-0.00	-0.00	0.4851	0.3750	0.1400	88.1	(2123K)

Appendix B

Troubleshooting

The following table lists common problems and their possible solutions.

Problem	Possible Cause(s)	Recommended Solution(s)
SpectraSuite starts, but does not show my spectrometer	1. The spectrometer is not plugged into the computer. 2. The attached spectrometer is not supported by SpectraSuite. 3. The device is not detected or identified.	1. Plug one end of the USB cable into the spectrometer, and the other end into the USB port of your computer. 2. See *USB Spectrometer and Device Control* for a list of spectrometers supported by SpectraSuite. 3. Disconnect any lamps or plug-ins that may be attached to the spectrometer, disconnect and reconnect the spectrometer, wait 10 seconds, and try again. If the spectrometer is detected, repeat with the lamp or plug-in connected. This may indicate a problem with an attached device. Under Windows and Linux, it is also possible that the spectrometer model may be newer than the driver file that informs the operating system about the spectrometer. The SpectraSuite update center does not yet update these system files, so it may be necessary to reinstall with the latest SpectraSuite installer to get the correct files.
SpectraSuite's splash window opens, but never finishes loading when attached to a USB2000 Spectrometer.	The USB2000 Spectrometer has firmware older than 2.41.0.	Use the **USB Programmer** and verify that the USB2000 has firmware version 2.41.0 or newer. The USB Programmer will also let you program a newer firmware if necessary.

Problem	Possible Cause(s)	**Recommended Solution(s)**
Some of the menu and toolbar items are grayed out (inactive).	Some menu and toolbar items require some action to be taken before they can be used.	Acquisition parameters, storing reference/dark spectra, and the Strip Chart require an unambiguous selection of an acquisition. If no acquisitions are running, try starting one. If more than one acquisition is started, try clicking on the desired trend in the graph to select the correct target. Similarly, try expanding the tree under the icon of the spectrometer and see how the controls respond to selecting each item. Right-click these items (or Control-click in MacOSX) to see additional actions for each. Minus dark requires a dark spectrum to be stored. A, T, R, and I (relative irradiance) require a reference and dark spectrum to be stored. Absolute Irradiance mode (I) requires a calibration and a stored dark spectrum. Photometry and energy/power/photons measurements require an active absolute irradiance calculation.
It took longer than expected to get a spectrum on the graph.	The host computer requested some change in the spectrometer's acquisition parameters (integration time, status of the strobe/lamp enable, etc.).	SpectraSuite discards the next spectrum it acquires after making changes to acquisition parameters. This extra discarded *stability scan* causes the next single-shot acquisition to take longer than normal because it is really acquiring two scans. For the same reason, a second external hardware trigger pulse may be required if the *Normal* free-running trigger mode is not being used. When preparing to do single-shot acquisitions or external triggering, it is recommended that all of the acquisition parameters be set in the continuously acquiring free-running mode to minimize this effect. If SpectraSuite is taking turns acquiring spectra with different acquisition parameters from the same spectrometer, it may be doing a stability scan before every sample scan. Also, as above, the number of scans to average is multiplied by the integration time.

Problem	Possible Cause(s)	Suggested Solution(s)
Can't access Absolute Irradiance mode	A spectrometer calibration and a Dark spectrum have not been stored.	Go to **File | New | New Absolute Irradiance Measurement** to open a wizard to guide you through the process. Absolute irradiance requires a spectrometer calibration (either loaded from disk or generated using a calibrated lamp) and a stored dark spectrum. The most typical reason for not being able to access absolute irradiance mode is that you must store a dark spectrum after loading a calibration.
The graph window shows a broken pattern of dots instead of a spectrum line.	On Microsoft Windows systems, ATI video cards are known to have problems displaying the graph properly.	Right-click the desktop, choose Properties, then select the Settings tab and click the **Advanced...** button. There should be a tab for the device that allows you to change the hardware acceleration. Set the hardware acceleration to about half and press **Apply**. That should immediately correct the problem. If not, try lowering the acceleration further.

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